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## Advisory Committee

<b>International</b>	Tom Gregorkiewicz (Universiteit van Amsterdam) Ajay Sood (Indian Institute of Science) Luke Lee (UC Berkeley) Huiming Cheng (Chinese Academy of Sciences)
<b>Domestic</b>	Sam Kyu Noh (Dongguk University) Hanjo Lim (Ajou University)

## Organizing Committee

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<b>Scientific Secretary</b>	Byoung Hee Moon (Sungkyunkwan University)
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# SCHEDULE

2019.01.20(Sun.)~2019.01.24(Thu.)

Time	Jan. 20	Jan. 21	Jan. 22	Jan. 23	Jan. 24
	Sun	Mon	Tue	Wed	Thu
9:00-9:20		Luke P. Lee	A.K. Sood	Hui-Ming Cheng	Maria C. Asensio
9:20-9:40					
9:40-10:00		Binghai Yan	Isabella Gierz	César Moreno	Tony Low
10:00-10:20					
10:20-10:40		Break (20m)	Break (20m)	Break (20m)	Break (20m)
10:40-11:00		Jun Sung Kim	L.V. Butov	Dinh Loc Duong	Søren Ulstrup
11:00-11:20		Kyung-Jin Lee		Gyung-Min Choi	
11:20-11:40		Christoph Renner	Gang Wang	Tim Wehling	Ki Kang Kim
11:40-12:00					Sung Wng Kim
					Closing Remark
12:10-13:40		Lunch (12:10-13:40)	Lunch (12:10-13:40)	Lunch (12:10-13:40)	
13:30-16:00	Registration	Discussion	Discussion	Discussion	
16:00-17:00	Tutorial-1 Paul S. Weiss				
17:00-17:20	Break (20m)				
17:20-18:20	Tutorial-2 Philip Kim	Dinner (17:30-19:00)	Dinner (17:30-19:00)	Break	
18:20-18:30	Break (10m)				
18:30-19:00	Welcome Reception (18:30-20:30)	Olga S. Ovchinnikova	Tom Gregorkiewicz	Banquet (18:30-21:30)	
19:00-19:20					
19:20-19:40		Kaihui Liu	Ji-Hee Kim		
19:40-20:00			Break		
20:00-20:20					
20:30-21:00		Poster-1 (20:30-22:30)	Poster-2 (20:30-22:30)		
21:00-21:30					
21:30-22:30					

# The 5<sup>th</sup> MUJU INTERNATIONAL Winter School Series

## SCIENTIFIC PROGRAM

January 20<sup>th</sup>, Sunday

13:30~16:00	Registration
16:00~17:00	<b>Tutorial Session I : Paul S. Weiss (Chair: Hyoyoung Lee)</b> "Precise chemical, physical, and electronic nanoscale contacts"
17:00~17:20	Break
17:20~18:20	<b>Tutorial Session II : Philip Kim (Chair: Sung Wng Kim)</b> "Atomic and electronic reconstruction at van der Waals interface in twisted 2D materials"
18:20~19:00	Break
19:00~21:00	Welcome Reception

January 21<sup>th</sup>, Monday

<b>Session I : Nanomaterials for Physics I (Chair: Seung Hyun Song)</b>	
09:00~09:40	<b>I-1 : Luke P. Lee</b> "Quantum biological electron transfer and its applications in life sciences and medicine"
09:40~10:20	<b>I-2 : Binghai Yan</b> "Topological materials: monopoles, surface states and more"
10:20~10:40	Break
<b>Session II : Nanomaterials for Physics II (Chair: Youngkuk Kim)</b>	
10:40~11:00	<b>I-3 : Jun Sung Kim</b> "Topological and ferromagnetic properties of iron-based van der Waals metals"
11:00~11:20	<b>I-4 : Kyung-Jin Lee</b> "Ferrimagnetic spintronics"
11:20~12:00	<b>I-5 : Christoph Renner</b> "Novel insight on the charge density wave ground state by scanning tunneling microscopy"
<b>Session III : Nanomaterials for Devices I (Chair: Heejun Yang)</b>	
19:00~19:40	<b>I-6 : Olga S. Ovchinnikova</b> "Towards atomically precise material fabrication: defect engineering of layered materials using focused ion beams"

19:40~20:20	<b>I-7 : Kaihui Liu</b> "Growth and application of meter-sized single-crystal graphene"
20:30~22:30	<b>Poster Session I</b>

## January 22<sup>th</sup>, Tuesday

<b>Session IV : Optical Properties of Nanomaterials I (Chair: Seong Chu Lim)</b>	
09:00~09:40	<b>I-8 : A.K. Sood</b> "Photophysics at nanoscale using time-resolved ultrafast spectroscopy"
09:40~10:20	<b>I-9 : Isabella Gierz</b> "Ultrafast materials design with tailored light pulses"
10:20~10:40	Break
<b>Session V : Optical Properties of Nanomaterials II (Chair: Jeongyong Kim)</b>	
10:40~11:20	<b>I-10 : L.V. Butov</b> "Indirect excitons in heterostructures"
11:20~12:00	<b>I-11 : Gang Wang</b> "Spin- and valley-phenomena, non-linear optics in atomically thin materials"
<b>Session VI : Optical Properties of Nanomaterials III (Chair: Hyun Seok Lee)</b>	
19:00~19:40	<b>I-12 : Tom Gregorkiewicz</b> "Optical properties of all-inorganic perovskite nanocrystals"
19:40~20:00	<b>I-13 : Ji-Hee Kim</b> "Zero excess energy for carrier multiplication in van der Waals layered materials"
20:30~22:30	<b>Poster Session II</b>

## January 23<sup>th</sup>, Wednesday

<b>Session VII : Nanomaterials for Devices II (Chair: Yunseok Kim)</b>	
09:00~09:40	<b>I-14 : Hui-Ming Cheng</b> "Graphene films and membranes: fabrication and applications"
09:40~10:20	<b>I-15 : César Moreno</b> "Atomically-precise graphene architectonics: 0D dots, 1D ribbons and 2D porous graphene"
10:20~10:40	Break

<b>Session VIII : Electronic and Magnetic Control of Nanomaterials (Chair: Dongseok Suh)</b>	
<b>10:40~11:00</b>	<b>I-16 : Dinh Loc Duong</b> "Room-temperature dilute magnetic semiconductor in V-doped monolayer WSe <sub>2</sub> "
<b>11:00~11:20</b>	<b>I-17 : Gyung-Min Choi</b> "Spin generation from charge current, heat, and light"
<b>11:20~12:00</b>	<b>I-18 : Tim Wehling</b> "Electronic correlations and pseudodoping in two-dimensional materials"
<b>18:30~21:30</b>	<b>Banquet</b>

**January 24<sup>th</sup>, Thursday**

<b>Session IX : Nano-Imaging and Light Manipulation (Chair: Mun Seok Jeong)</b>	
<b>09:00~09:40</b>	<b>I-19 : Maria C. Asensio</b> "Electronic and chemical nano-imaging of 2D materials beyond graphene"
<b>09:40~10:20</b>	<b>I-20 : Tony Low</b> "Manipulating light flow with 2D materials plasmons"
<b>10:20~10:40</b>	Break
<b>Session X : Nanomaterials for Devices III (Chair: Young Min Kim)</b>	
<b>10:40~11:20</b>	<b>I-21 : Søren Ulstrup</b> "Electronic structure and ultrafast dynamics of chalcogenide heterolayers"
<b>11:20~11:40</b>	<b>I-22 : Ki Kang Kim</b> "Toward single-crystal 2D materials on wafer scale"
<b>11:40~12:00</b>	<b>I-23 : Sung Wng Kim</b> "Discovery of new two-dimensional van der Waals materials: layered Zintl phases"
<b>12:00~12:20</b>	<b>Closing Remark</b>

# The 5<sup>th</sup> MUJU INTERNATIONAL Winter School Series

## POSTER SESSION

January 21<sup>th</sup>, Monday

No.	Name	Title
PM-1	Bing Deng	Graphene as electronic materials: controlled growth of single-crystal graphene wafer
PM-2	Luzhao Sun	Visualizing the fast growth of large single-crystalline graphene
PM-3	Xian-Gang Hu	Fabricating high-efficiency silicon heterojunction solar cells with small-bundle single-wall carbon nanotubes
PM-4	Zhepeng Zhang	Epitaxial growth of 2D metallic VSe <sub>2</sub> single crystals and their heterostructures with semiconducting MX <sub>2</sub>
PM-5	Woo-Sung Jang	Directional distribution of metal interstitials in Nb <sub>2</sub> Se <sub>3</sub> compound
PM-6	Lingxiang Qin	Mesoporous graphene frameworks and its application in VOCs adsorption
PM-7	Wonoh Lee	Carbon fabric-based flexible supercapacitors with polydopamine-coated 3D carbon nanostructures
PM-8	Jia Guo	Synthesis of hierarchical tree-like few-layered MoS <sub>2</sub> nanosheets anchored on vertically aligned carbon nanotube networks
PM-9	Gyawali Ghanashyam	Electrochemical performance of poly sodium 4-styrenesulfonate intercalated thermally reduced graphite oxide paper for supercapacitors
PM-10	Aryal Krishna Prasad	Functionalization of thermally reduced graphite oxide and carbon nanotubes by p-sulfonatocalix[4]arene and supramolecular recognition of tyrosine
PM-11	Thuy Thi Tran	Characterization of iron cerium oxide (FeCeO <sub>x</sub> ) nanoparticles prepared by hydrothermal synthesis for hydrogen sulfide (H <sub>2</sub> S) removal application
PM-12	Young-Hoon Kim	Hierarchically-structured core-shell design of a lithium transition metal oxide cathode material for excellent electrochemical performance
PM-13	Olaniyan Ibukun	Titanium dioxide- molybdenum disulfide for photocatalytic degradation of methylene blue
PM-14	Wooseon Choi	Quantification reliability of ADF-STEM imaging for vacancy concentration in 1L-TMDs
PM-15	Meeree Kim	Ligand exchange of colloidal WSe <sub>2</sub> : counter cation-dependent hydrogen evolution reaction (HER) study
PM-16	Thi Anh Le	Intertwined titanium carbide MXene within 3D tangled polypyrrole nanowires matrix for enhanced Supercapacitor Performances
PM-17	Soyeong Kwon	Fabrication and characterizations of MoS <sub>2</sub> /Au nanogratings
PM-18	Xu Wei	Toward ultraclean 2D heterostructure interfaces: h-BN as a novel tool to visualize organic residues
PM-19	Doyoung Kim	Carbon-based asymmetric capacitor for high-performance energy storage devices
PM-20	Hyunjung Kim	Colloidal synthesis of hexagonal FeIn <sub>2</sub> S <sub>4</sub> and its layer dependent band structures
PM-21	Vu Thi Oanh	Non-enzymatic glucose sensor based on CuO nanoparticles modified screen-printed carbon ink electrode
PM-22	Ngoc Quang Tran	Ultralight and flexible sodium titanate nanowire aerogel with superior sodium storage

<b>PM-23</b>	<b>Vo Thanh Duoc</b>	Fabrication of hydrogen gas sensor based on SnO <sub>2</sub> /Pt thin film on Kapton substrate
<b>PM-24</b>	<b>Jing Wu</b>	Engineering on Ni-Co-S bifunctional electrocatalyst for water-splitting
<b>PM-25</b>	<b>Huong Thi Diem Bui</b>	Theoretical insights into the size-dependent Ru clusters on N-doped graphene for electrocatalytic hydrogen evolution and oxygen reduction reactions
<b>PM-26</b>	<b>Amol R. Jadhav</b>	Molecularly ultrathin sheets of Fe-graphene on nickel foam supported NiCo <sub>2</sub> O <sub>4</sub> microrod arrays as a highly efficient bifunctional electrocatalyst for oxygen and hydrogen evolution reaction
<b>PM-27</b>	<b>Soo Ho Choi</b>	Intercalates-assisted electrochemical transfer of monolayer WS <sub>2</sub> film on gold substrate
<b>PM-28</b>	<b>Suicai Zhang</b>	Graphdiyne nanowall for enhanced photoelectrochemical performance of Si heterojunction photoanode
<b>PM-29</b>	<b>Stephen Boandoh</b>	Wafer-scale van der Waals heterostructures with ultraclean interfaces via the aid of viscoelastic polymer
<b>PM-30</b>	<b>Mengyu Hong</b>	Influence of indium doping on dissolving behavior and stability of quasi-2D ZnO nanobelts in solution
<b>PM-31</b>	<b>Ashwani Kumar</b>	Activating the dull bimetallic phosphide via copper nanowire insertion towards efficient hydrogen evolution reaction
<b>PM-32</b>	<b>Se Hwang Kang</b>	Oxidation-resistive two-dimensional dihafnium sulfide electride with efficient electrocatalytic activities in water-based solution
<b>PM-33</b>	<b>Hee Min Hwang</b>	Dual function of metal doped B-TiO <sub>2</sub> without hole scavenger for complete degradation of nerve agent
<b>PM-34</b>	<b>Suresh Vasimalla</b>	Visible light mediated C-C bond formation by a single Blue TiO <sub>2</sub> based photo-chiral catalyst
<b>PM-35</b>	<b>Sora Bak</b>	Role of phase-selective defects in TiO <sub>2</sub> on organic photoreaction under visible light
<b>PM-36</b>	<b>Kyungwha Chung</b>	Inherently negatively charged copper nanoparticles with oxidation resistance
<b>PM-37</b>	<b>Woo Hyun Han</b>	Green phosphorus with high mobility and tunable direct band gap
<b>PM-38</b>	<b>Hongdan Wang</b>	Possibility to find enantiomeric excess in organic reactions by using circularly polarized light
<b>PM-39</b>	<b>Jianmin Yu</b>	Solution processable ReS <sub>2</sub> -molecular Z-scheme-TiO <sub>2</sub> for excellent solar hydrogen generation by fast charge transfer through multiple junctions
<b>PM-40</b>	<b>Min Seok Kim</b>	The effect of Li and Ag intercalation to MoS <sub>2</sub> for memory device
<b>PM-41</b>	<b>Liu Yang</b>	Dual vacancies engineering of 2D MnO <sub>2</sub> for overall water splitting
<b>PM-42</b>	<b>Anand P. Tiwari</b>	Chemical strain formation through anion substitution in ternary transition metal chalcogenides for efficient hydrogen evolution reaction
<b>PM-43</b>	<b>Sara Ajmal</b>	Hole scavenger-free photocatalytic H <sub>2</sub> Evolution on highly uniform 'Pt' sub-nanoclusters embedded on partially disordered blue TiO <sub>2</sub>
<b>PM-44</b>	<b>Byung Il Yoo</b>	Birch reduction of aromatic compounds by inorganic electride [Ca <sub>2</sub> N] <sup>+</sup> •e <sup>-</sup>
<b>PM-45</b>	<b>Dae Young Park</b>	Large area sputtered ReS <sub>2</sub> film for optoelectronics
<b>PM-46</b>	<b>Jinbong Seok</b>	Studies of electrochemically deposited Platinum on MoTe <sub>2</sub> for catalytic behavior
<b>PM-47</b>	<b>Zhiyang Zeng</b>	Nanoporous graphene membrane for separation
<b>PM-48</b>	<b>Jinsun Lee</b>	The synergistic effect of nitrogen fixation over partially reduced titanium dioxide For solar-driven nitrogen conversion to ammonia
<b>PM-49</b>	<b>Yonas Assefa Eshete</b>	Heterophase homojunction in single crystal MoTe <sub>2</sub> for enhanced catalytic performance



<b>PM-50</b>	<b>Ning Ling</b>	Hydrogen bubble-assisted synthesis of reduced graphene oxide-WTe <sub>2</sub> hybrid catalyst for hydrogen evolution
<b>PM-51</b>	<b>Won Tae Kang</b>	Direct growth of doping controlled monolayer WSe <sub>2</sub> by selenium-phosphorus substitution
<b>PM-52</b>	<b>Jae Hyeon Ryu</b>	Wafer scale continuous bilayer graphene films synthesis by using inductively coupled plasma - chemical vapor deposition
<b>PM-53</b>	<b>Ganesh Ghimire</b>	Study of defect on atomically thin ReS <sub>2</sub> through chemical treatment effect
<b>PM-54</b>	<b>Shrawan Roy</b>	Microscopic origin of vacancy healing in two-dimensional semiconductors via chemical treatment
<b>PM-55</b>	<b>Ho Beom Jeon</b>	Fabrication of perovskite films using solvent engineering with CsPbBr <sub>3</sub> seed crystallization
<b>PM-56</b>	<b>Chau T. K. Nguyen</b>	Blue TiO <sub>2</sub> /WO <sub>3</sub> /Ag hybrid nanostructures for solar light-driven CO <sub>2</sub> reduction into 100% CO
<b>PM-57</b>	<b>Jeong-Gyun Kim</b>	Carbon-nanotube based hybrid composite superconducting wire
<b>PM-58</b>	<b>Joosung Kim</b>	The effect of alcohol solvent on the synthesis of MoS <sub>2</sub> quantum dots with solvothermal method
<b>PM-59</b>	<b>Bong Ho Kim</b>	Large-area and low-temperature synthesis of few-layered WS <sub>2</sub> films for photodetectors
<b>PM-60</b>	<b>Mondal Shuvra</b>	TMDs-assisted graphene foam/polymer hybrid nano-structures for wearable strain-pressure sensor
<b>PM-61</b>	<b>Soon Hyeong Kwon</b>	Microstructural evolution of sputtered SnS <sub>2</sub> , SnS thin films by room temperature electron beam irradiation
<b>PM-62</b>	<b>Pengfei Yang</b>	Wafer-scale few-layer molybdenum disulfide as a multifunctional optical material
<b>PM-63</b>	<b>Hyun Kim</b>	Direct growth of layered antimonene on transition metal dichalcogenides by chemical vapor deposition
<b>PM-64</b>	<b>Thi Suong Le</b>	Quantum dots embedded hexagonal iron oxide for fiber-shaped battery-like anode
<b>PM-65</b>	<b>Thi Hoai Thuong Luu</b>	A free-standing SnS <sub>2</sub> nanoparticles/CNT thin film for sodium ion battery anode electrode
<b>PM-66</b>	<b>Yunhee Cho</b>	CsPbBr <sub>3</sub> @metal nanocrystals for photocatalytic application
<b>PM-67</b>	<b>Hanchul Kim</b>	Energetics and bias-dependent scanning tunneling microscope images of intrinsic defects in 2H-MoTe <sub>2</sub>
<b>PM-68</b>	<b>Sung-Gyu Lee</b>	Flexible broadband Cr/PET/Cr solar absorber
<b>PM-69</b>	<b>Hyang Mi Yu</b>	Degradation analysis of perovskite films using the photo thermal induced resonance spectroscopy
<b>PM-70</b>	<b>Jong Gil Park</b>	Multi-functional aligned carbon nanotubes sheet for liquid crystal display device
<b>PM-71</b>	<b>Theophile Niyitanga</b>	Thermally Reduced Graphite oxide/Carbon Nanotubes Supported Molybdenum Disulfide as Catalysts for Hydrogen Evolution Reaction
<b>PM-72</b>	<b>Joo Song Lee</b>	Wafer-scale single-crystal hexagonal boron nitride film via self-collimated grain formation
<b>PM-73</b>	<b>Farman Ullah</b>	Growth and Simultaneous valleys Polarization of Monolayered MoSe <sub>2</sub> -WSe <sub>2</sub> lateral heterostructure

January 22<sup>th</sup>, Tuesday

No.	Name	Title
PT-1	Jing Liang	Monitoring local strain vector in atomic layered $\text{MoSe}_2$ by second-harmonic generation
PT-2	Shun Feng	Multilayer $\text{MoS}_2$ field-effect transistors using 2-dimensional $\alpha\text{-Mo}_2\text{C}$ film as electrodes
PT-3	Bo Li	High-performance phototransistors based on a hybrid channel of $\text{CsPbBr}_3$ quantum dot and carbon nanotube network
PT-4	Jing Chen	Designing nanoscale elastic structures of 2D materials-based electrodes
PT-5	Jun Suk Kim	Unusual K-point phonons in noble metal/graphene heterostructure
PT-6	Youngkuk Kim	$Z_2$ monopole nodal lines and the Stiefel-Whitney insulator in the ABC graphdiyne
PT-7	Youngjo Jin	Coulomb drag behavior in graphene/ $\text{MoS}_2$ heterointerface
PT-8	Chinh Tam Le	Spin orbit engineered resonant second harmonic generation of artificially stacked Van der waal multilayers
PT-9	Doan Viet Truong	Simulation and study of the influence of the hole selective contact, buffer intrinsic layer, densities of interface defects, and transparent conductive oxide on TMO/c-Si heterojunction solar cell
PT-10	Minh Dao Tran	Two-terminal multibit optical memory via van der Waals heterostructure
PT-11	Subash Adhikari	Bandgap renormalization in $\text{CsPbBr}_3$ perovskite quantum Dot/ $\text{MoS}_2$ heterostructure via charge transfer at room temperature
PT-12	Hye-Jin Jin	Interplay of free charges of 2D van der Waals materials with the large polarization of ferroelectric oxides: a clue to photo-memristors
PT-13	Dinh Hoa Luong	Enhanced light-matter interactions in self-assembled plasmonic nanoparticles on 2D semiconductors
PT-14	Jinbao Jiang	Ultra-short vertical-channel 2D transistors
PT-15	Sidi Fan	Tunable negative differential resistance in van der Waals heterostructures at room temperature by tailoring interface
PT-16	Junhong Na	Negative differential resistance in few-layer black phosphorus/ $\text{SnSe}_2$ heterostructure
PT-17	Changjiu Teng	Gate-tunable memory synaptic photomemristor based on two-dimensional transition metal di-chalcogenide
PT-18	Eunah Kim	Optical absorption enhancement in 2D $\text{MoS}_2$ monolayers: influences of interference and 3D dielectric material refractive index
PT-19	Youngbum Kim	Near-field imaging of charge separation and transfer at $\text{MoSe}_2$ - $\text{WSe}_2$ lateral heterojunction
PT-20	Yashar Mayamei	Electrical characterization of graphene nanoribbon on h-BN
PT-21	Lei Li	RF Characterization and modeling of black phosphorus MOSFETs
PT-22	Yongjun Lee	Bright light emission by suppressed exciton-exciton annihilation in monolayer $\text{WS}_2$ by laser irradiation
PT-23	Yang Ou	Edge introduced barrier in $\text{MoS}_2$ - $\text{WS}_2$ van der Waals heterojunctions

<b>PT-24</b>	<b>Yong Ju Yun</b>	Multifunctional reduced graphene oxide based electronic textiles for wearable electronic/optoelectronic applications
<b>PT-25</b>	<b>Yong Ju Yun</b>	Highly stretchable and biocompatible porous reduced graphene oxide films toward epidermal electronics
<b>PT-26</b>	<b>Jongho Park</b>	Ferromagnetic heavy fermion system with non-fermi liquid behavior in antiperovskite $\text{Gd}_3\text{SnC}$
<b>PT-27</b>	<b>Simgeon Oh</b>	Energy band modulation to improve HER performance by phase selective reduction of $\text{TiO}_2$
<b>PT-28</b>	<b>Ho Min Choi</b>	Edge contact for carrier injection and transport in $\text{MoS}_2$ field-effect transistor
<b>PT-29</b>	<b>Thanh Luan Phan</b>	A high on/off ratio of top gate ZnO thin films transistors array with a buffer layer of self-assembled monolayer of molecule
<b>PT-30</b>	<b>Seung Yong Lee</b>	Quasi-atomic electrons in two-dimensional ferromagnetic electride
<b>PT-31</b>	<b>Michael Neumann</b>	Noise nanospectroscopy as a probe for defect dynamics in monolayer $\text{MoS}_2$
<b>PT-32</b>	<b>Yong Seon Shin</b>	Mobility engineering in the vertical field effect transistor based on van der Waals heterostructures
<b>PT-33</b>	<b>Junseong Song</b>	Discovery of two-dimensional van der Waals Zintl phase and bidimensional polymorphism of $\text{ZnSb}$
<b>PT-34</b>	<b>Hyun Yong Song</b>	Ferromagnetic two-dimensional van der Waals electride
<b>PT-35</b>	<b>Young Rae Kim</b>	Application for high sensitive proximity sensor with CVD-growth $\text{MoS}_2$
<b>PT-36</b>	<b>Ui Yeon Won</b>	Very high open-circuit voltage in dual-gate graphene/silicon heterojunction solar cells
<b>PT-37</b>	<b>Ilmin Lee</b>	High responsivity, fast molybdenum disulfide photo-transistor using tunable schottky barrier
<b>PT-38</b>	<b>Kye Whan Cho</b>	High performance graphene photodetector with van der Waals heterostructure through tuning carrier tunneling
<b>PT-39</b>	<b>Chanwoo Lee</b>	Unveiling defect-related raman mode of monolayer tungsten disulfide via tip-enhanced resonance raman scattering
<b>PT-40</b>	<b>Hayoung Ko</b>	2D Heterostructure for enhanced gas barrier performance via synergetic effect
<b>PT-41</b>	<b>Duc Anh Nguyen</b>	Highly enhanced photoresponsivity of monolayer $\text{WSe}_2$ photodetector with nitrogen-doped graphene quantum dots
<b>PT-42</b>	<b>Dohyun Kim</b>	Thermal-driven electronic band change in layered semimetallic $\text{MoTe}_2$
<b>PT-43</b>	<b>Sera Kim</b>	Layer-decoupling and stacking order modulation of multi-layered graphene by electride-based electron injection
<b>PT-44</b>	<b>Isabella Gasparutti</b>	Ultraclean van der Waals heterostructure assembly with unity yield by solvent-assisted polydimethylsiloxane stamping
<b>PT-45</b>	<b>Dongyeun Won</b>	Polymorphic 2D charge density waves in $\text{VTe}_2$
<b>PT-46</b>	<b>Chulho Park</b>	Development of P-N diode in few-layer $\text{ReS}_2/\text{WSe}_2$ stacking structure
<b>PT-47</b>	<b>Ngoc Thanh Duong</b>	Thickness-dependent functionality of $\text{MoS}_2/\text{MoTe}_2$ van der Waals heterostructure
<b>PT-48</b>	<b>Jung Ho Kim</b>	All-optical logic devices via plasmon-exciton interconversion

<b>PT-49</b>	<b>Nahee Park</b>	Analysis of anomalous behavior at ferroelectric/two-dimensional material interface
<b>PT-50</b>	<b>Van-Tam Nguyen</b>	Significantly enhanced electromagnetic interference shielding effectiveness in graphene porous network with Fe <sub>3</sub> O <sub>4</sub> nanoparticles-intercalated 2D Ti <sub>3</sub> C <sub>2</sub> Mxene
<b>PT-51</b>	<b>Gwanmu Lee</b>	Graphene/PMN-PT field effect transistor with interdigitated electrode
<b>PT-52</b>	<b>Geunwoo Hwang</b>	A tunneling device for optoelectronic application with near-infrared light: Au/h-BN/MoTe <sub>2</sub> tunneling device study
<b>PT-53</b>	<b>Joonggyu Kim</b>	Hall magnetic sensor based on two-dimensional van der Waals materials
<b>PT-54</b>	<b>Kyungrok Kang</b>	Temperature-driven Lifshitz transition triggering non-Fermi liquid behavior in semimetal Nb <sub>2</sub> Se <sub>3</sub>
<b>PT-55</b>	<b>Yourack Lee</b>	Continuous thermopower from capillary-induced carbon nanotube yarn Thermoelectric Candle
<b>PT-56</b>	<b>Hyeonbeom Kim</b>	Charge trap effect at graphene channel caused by strong electrical affinity of fluorine
<b>PT-57</b>	<b>Dongseok Shin</b>	Plasma treatment induced n-type doping effect on few-layer WSe <sub>2</sub> field-effect transistors
<b>PT-58</b>	<b>Jin Cheol Park</b>	Real bandgap investigation of CVD grown 1T'-MoTe <sub>2</sub> via infra-red spectroscopy
<b>PT-59</b>	<b>Tuan Khanh Chau</b>	Unusual quantum hall effect across graphene grain-boundary grown by chemical vapor deposition
<b>PT-60</b>	<b>Hojoon Yi</b>	Thermal conductivity of metal-coated carbon fibers
<b>PT-61</b>	<b>Hamza Zad Gul</b>	Presence of photothermal and photoelectric in partially suspended PtSe <sub>2</sub>
<b>PT-62</b>	<b>Won Kil Sakong</b>	Broadband photoresponse of multi-layer MoS <sub>2</sub> from ultraviolet to infrared through metal-insulator transition
<b>PT-63</b>	<b>Dang Xuan Dang</b>	The broad range pressure detection by electro-thermal response of metal-coated carbon fiber
<b>PT-64</b>	<b>Sungyu Park</b>	Transport characteristics of van der Waals junction assembled with NbSe <sub>2</sub> and FeSe
<b>PT-65</b>	<b>H. C. Jeon</b>	Electronic and optical properties of staggered ZnO/ZnO <sub>1-x</sub> S <sup>x</sup> -ZnO <sub>1-y</sub> S <sub>y</sub> /ZnO quantum well for bluish-green light-emitting diodes
<b>PT-66</b>	<b>Ngoc Quang Tran</b>	Anion-cation double substitution in transition metal dichalcogenide to accelerate water dissociation kinetic for electrocatalysis
<b>PT-67</b>	<b>Seungho Bang</b>	Augmented quantum yield of a 2D monolayer photodetector by surface plasmon coupling
<b>PT-68</b>	<b>Hyeon Jun Jeong</b>	Organometal halide perovskite to optoelectronic devices fabricated with homogeneous Nano-seed
<b>PT-69</b>	<b>Juchan Lee</b>	High peak-to-valley current ratio in SnSe <sub>2</sub> /MoTe <sub>2</sub> tunnel diode
<b>PT-70</b>	<b>Bora Kim</b>	2-D Transition metal dichalcogenides charge transport layers for perovskite solar cells
<b>PT-71</b>	<b>Ji Eun Kim</b>	Highly sensitive graphene biosensor by monomolecular self-assembly of receptors on graphene surface
<b>PT-72</b>	<b>Yang Wang</b>	SWCNT/h-BN heterostructures: fabrication, interface and transport properties
<b>PT-73</b>	<b>Marco van der Laan</b>	Coexistence of indirect- and direct-bandgap excitons in monolayer WSe <sub>2</sub>

# ***Abstract***

## **Invited Session**

- Tutorial Session (T)
- Invited Talks (I)

## Precise chemical, physical, and electronic nanoscale contacts

**Paul S. Weiss**

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The physical, electronic, mechanical, and chemical connections that materials make to one another and to the outside world are critical. Just as the properties and applications of conventional semiconductor devices depend on these contacts, so do nanomaterials, many nanoscale measurements, and devices of the future. We discuss the important roles that these contacts can play in preserving key transport and other properties. Initial nanoscale connections and measurements guide the path to future opportunities and challenges ahead. Band alignment and minimally disruptive connections are both targets and can be characterized in both experiment and theory. I discuss our initial forays into this area in a number of materials systems [1,2].

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# Atomic and electronic reconstruction at van der Waals interface in twisted 2D Materials

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Control of the interlayer twist in the vdW interface has been widely used to engineer an artificial 2-dimensional (2D) electronic systems by the formation of a moiré superlattice. Many exotic physical phenomena occur associated with the incommensurability of the moiré superstructures; the fractal energy spectrum of Hofstadter butterfly and recently discovered Mott insulating and unconventional superconducting behavior of the ‘magic’ twist angle bilayer graphene have demonstrated the wealth of the nontrivial topology of electronic band structures. However, the atomic scale microstructures and electronic structures of vdW interfaces have been understood in the frame of rigid rotational moiré structures without atomic scale relaxation. In this presentation, we will discuss the engineered atomic scale reconstruction at twisted vdW interface [1]. We find that the vdW interaction energy that favors interlayer commensurability competes against the intralayer elastic lattice distortion to form a quasi-periodic domain structure, inducing profound changes in electronic structure. Particularly, we show quantitative analysis of the engineered atomic-scale reconstruction completely controlled by the twist angle between two graphene layers and anomalous electron transport occurring in the network of topologically protected propagation modes along the domain boundaries. Interfaces between vdW materials are a crucial material platform for realization of novel quantum electronics. Our discoveries of atomic scale reconstruction at vdW interfaces will provide a new route to engineer the 2D materials for exceptional functionalities.

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# Quantum biological electron transfer and its applications in life sciences and medicine

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Electron transfer (ET) essentially involves in virtually all biological processes such as photosynthesis, cellular respiration, DNA repair, cellular homeostasis, cell death, cancer, neurodegenerative diseases, etc. In particular, ET in between biological molecules and cytochromes in mitochondria plays a vital role in the process of cell life and death. However, there is no real-time imaging method to capture spatiotemporal ET dynamics in living cells to date. In this talk, I will present the quantum biological electron tunneling (QBET) junction and its applications in *in vivo* ET imaging of living cells and *in vitro* molecular diagnostics. For the exploration of cellular galaxy, we created *in vivo* nanosatellites using QBET junctions, which are formed by resonant optical antennas, barriers, and cytochromes. These QBET junctions allow us to see not only ET dynamics of enzymes in live cells, but also the mechanism of cytochromes in mitochondrial control of cellular apoptosis and necrosis, which might shed new light on the treatments of cancer or neurodegenerative diseases. For *in vitro* molecular diagnostics, QBET junctions can create ultrafast photonic PCR on chip and form integrated molecular diagnostic systems (iMDx). In order to accomplish low-cost rapid precision molecular diagnostics, our iMDx are established with three key elements of precision medicine: (1) ultrafast photonic PCR for the early detection of DNA and RNA biomarkers and signal amplifications of protein markers, (2) a self-contained sample preparation from whole blood that allows a sample-to-answer readout platform, (3) interactive e-healthcare IT with smart analytics. If time permits, I will also discuss microphysiological analysis platforms (MAP), or organoids on chip, which provides a solution to form physiologically relevant models of organoids with the capability of non-invasive real-time monitoring for patient-oriented precision drug screening and mini-brains MAP for understanding ET in mitochondria and mitochondrial dysfunction in neurodegenerative diseases.



# Topological materials: monopoles, surface states and more

**Binghai Yan**

*Weizmann Institute of Science, Israel*

The classification and discovery of topological materials have attracted intensive research attention in the past decade. After explaining basic concepts of the topological states, I will introduce our most recent progress on novel topological states discovered in a well-known family of materials, transition metal dichalcogenides. Beyond surface states, the topology also brings exotic transport phenomena, such as a nonlinear version of the Hall effect (verified by recent experiments), but without breaking the time-reversal symmetry.

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## **Topological and ferromagnetic properties of iron-based van der Waals metals**

**Jun Sung Kim**

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Topological semimetals, new states of matters whose low energy electronic structure possesses several band contact points or lines, are generally expected to exhibit intriguing topological responses. Up to now, most of the studies on topological semimetals are limited to non-magnetic materials with time-reversal symmetry. However, magnetic materials can also be endowed with topological band structures in which the interplay of magnetism and band topology can generate novel correlated topological phenomena. In this talk, I will introduce iron-based van der Waals (vdW) materials, where combination of magnetism, spin-orbit interaction, and topological band structures gives rise to unusual physical properties and magnetic tunability [1,2]. This demonstrates that topological and ferromagnetic vdW materials have great potential for various spin-dependent electronic functionalities

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## Ferrimagnetic spintronics

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Spintronics is a multidisciplinary field whose central theme is the active manipulation of spin degrees of freedom in solid-state systems. The core magnetic system for spintronics research has been ferromagnets since they serve as spin-polarizers/detectors and offer non-volatile memory and logic technologies. Recently, much effort has been expended in employing antiferromagnets and ferrimagnets as core elements in spintronic applications because of their fast dynamics. This talk will discuss the underlying mechanism of fast dynamics of compensated and uncompensated staggered moments, driven by magnetic fields or spin-transfer torques [1-5].

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# Novel insight on the charge density wave ground state by scanning tunneling microscopy

**Christoph Renner**

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Charge density wave (CDW) phases permeate the phase diagram of many correlated electron systems. Despite decades of research, CDWs are still lacking a detailed understanding. There is renewed interest in CDWs motivated by the possible competition of this quantum phase with superconductivity, in particular in high temperature superconductors. Moreover, robust evidence for nesting at the Fermi level, the preferred mechanism, is firmly established only in very few CDW systems, while the nature and amplitude of the associated gap in the band structure remain largely unsettled. We will discuss recent scanning tunneling microscopy and spectroscopy experiments providing novel insight on the CDW phase observed in transition metal dichalcogenides (TMDs). After a brief review of some open issues in selected CDW systems, we discuss unique investigation opportunities offered by the recent developments preparing exfoliated TMDs of variable thicknesses, from bulk to monolayer. We find a striking non-monotonic thickness dependence of the CDW phase transition temperature ( $T_{\text{CDW}}$ ) in  $\text{VSe}_2$  [1].  $T_{\text{CDW}}$ , determined directly from the charge modulation amplitude imaged by STM, is found to diminish with thickness above 20nm. Meanwhile, below 10nm thickness,  $T_{\text{CDW}}$  is increasing to exceed the bulk values by nearly 40% in the thinnest specimen. Although a detailed theoretical understanding is yet to be developed, this behavior reflects a 3D to 2D dimensional crossover followed by quantum confinement in the thinnest samples. Next, we introduce a powerful real space fitting procedure, allowing us to map the full complex CDW order parameter with a spatial resolution of the order of half a CDW period. Thus obtained images of the local amplitude, phase and wavelength provide unprecedented insight into the CDW ground state. We find in particular that the CDW in TMDs consists of three individual components. Phase contrast images reveal domain walls, discommensurations and topological defects such as vortices and vortex anti-vortex pairs in each of the three components. Finally, we show how the atomic resolution capabilities of scanning probe imaging [3] gives insight into the three dimensional real space structure of the CDW reconstruction.

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## **Towards atomically precise material fabrication: defect engineering of layered materials using focused ion beams**

**Olga S. Ovchinnikova**

*Chemical Imaging Team Lead and R&D Scientist*

*Center for Nanophase Materials Sciences*

*Oak Ridge National Laboratory*

The scalability of electronic and information technology devices depends on the ability to tune layered materials. With the recent development of CVD-growth processes for high quality 2-dimensional materials, large scale fabrication of these materials is become routine. However, critical is the structuring and functional tuning of these materials, as currently being done for semiconductors. Here, I will discuss the use of focused helium ion beams in tailoring the functionality of 2D materials including graphene, dichalcogenides and copper indium thiophosphate (CIPS) with nanometer precision. Using a helium ion beam under high dosing allows for milling and structuring of devices with nanometer precision and prevents ion implantation and resist contamination effects. For lower helium ion doses we are able to tune the mobility as ascertained by local transport measurements. The nature of the associated properties of this material were explored using a combination of aberration-corrected scanning transmission electron microscopy (STEM), scanning probe microscopy (SPM) and optical spectroscopy and mass spectrometry techniques that provided insight into local mechanical, electromechanical, chemical and atomic structure properties of these devices and elucidate the effect of ion beam dose on device performance. Future perspective and scalability of this approach to device fabrication will also be discussed.

## Growth and application of meter-sized single-crystal graphene

**Kaihui Liu**

*School of Physics, Peking University, Beijing, China*

Graphene is of only one atomic layer thick and its property is therefore very sensitive to the interfacial interaction with other materials. By designing and utilizing this interfacial interaction, we have lots of opportunity in engineering the growth and applications of graphene. In this talk I will introduce several our recent works on this topic, including ultrafast graphene growth [1, 2], epitaxial meter-sized single-crystal graphene growth [3], and ultrafast broadband charge collection [4].

**Key words:** Graphene, Growth, Physics

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## **Photophysics at nanoscale using time-resolved ultrafast spectroscopy**

**A.K. Sood**

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Ultrafast lasers offer unique possibilities to control and probe transient processes in nano materials. Following photoexcitation by a femtosecond laser pulse, the carrier dynamics includes many important processes like thermalization, energy relaxation, exciton formation and spin dynamics which are impacted by dimensionality. Their understanding is crucial not only for many optoelectronic applications, but also to gain a deeper understanding of physical processes in nano-materials. My talk will discuss some of our recent work on the dynamics of optical pump induced photocarriers in single and bilayer graphene, graphane (hydrogen functionalized graphene) and carbon nanotubes as probed by time-resolved optical pump-terahertz probe spectroscopy.

Our recent ongoing work on tunable Plasmon-assisted generation of hot carriers in graphene on an ultrathin gold film with periodic array of holes (showing anomalous transmission resonances) as probed by ultrafast time-resolved differential reflectance will also be discussed.

# Ultrafast materials design with tailored light pulses

**Isabella Gierz**

*Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany*

The electronic properties of solids are mainly determined by the orbital overlap between neighbouring atoms. Therefore, electronic properties are commonly controlled via the chemical composition that determines the relevant structural parameters such as bond angles and lengths.

My group follows a different approach where control of the effective orbital overlap is achieved by periodic modulation of the solid with strong laser fields in the (mid-)infrared spectral range. We investigate the resulting band structure changes with time- and angle-resolved photoemission spectroscopy (tr-ARPES).

The stable crystal structure and therefore the band structure of a solid is determined by the deepest minimum on the potential energy surface. We follow three different approaches to modify the shape of the potential energy surface with light and thereby control the electronic properties of different low-dimensional materials:

I will present results on the light-induced insulator-to-metal phase transition in one-dimensional indium wires where strong electronic excitation quenches the minimum on the potential energy surface associated with the insulating ground state [1,2].

Next I will show how resonant driving of an infrared-active lattice vibration in bilayer graphene results in a transient enhancement of the electron-phonon coupling constant [3,4].

Recently, coherent modulation of the Bloch electron's momentum with strong light fields has emerged as a new route for dynamical band structure engineering. There are predictions for various light-induced phase transitions including the formation of Floquet topological insulators [5] and Mott insulating states [6]. I will present our recent results concerning the observation of photon-dressed states in graphene and bulk WSe<sub>2</sub> and end with an outlook on future projects.

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## Indirect excitons in heterostructures

**L.V. Butov**

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An indirect exciton (IX), aka interlayer exciton or charge transfer exciton, is a bound pair of an electron and a hole confined in spatially separated layers.

Due to their long lifetimes, IXs can cool below the temperature of quantum degeneracy. This gives an opportunity to realize and study cold excitons. We will present direct measurements of spontaneous coherence and Bose-Einstein condensation of IXs. We will present phenomena observed in the IX condensate, including the commensurability effect of exciton density wave, spin textures, and Pancharatnam-Berry phase and long-range coherent spin transport.

IXs are dipoles and their energy can be controlled by voltage. This gives an opportunity to build devices, which operate with excitons in place of electrons. We will present excitonic devices, including excitonic transistor, trap, lattice, conveyer, ramp, storage, and split-gate devices.

We will present van der Waals heterostructures where IX condensation can be realized at high temperatures. We will present IXs at room temperature in van der Waals heterostructures.

# Spin- and valley-phenomena, non-linear optics in atomically thin materials

**Gang Wang**

*G. Soavi<sup>1</sup>, M. Barbone<sup>1,2</sup>, B. Urbaszek<sup>3</sup>, X. Marie<sup>3</sup>, M. Atatüre<sup>2</sup>, A. C. Ferrari<sup>1</sup>*

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Atomically thin materials are a promising platform for optoelectronics and spin/valley related phenomena, due to their reduced dimensionality, crystal symmetry and the possibility to arrange them in heterostructures. In semiconducting monolayer transition metal dichalcogenides (TMDs), due to the missing inversion symmetry and strong spin-orbit interaction, spin and valley degrees of freedom are coupled [1]. The resulting valley dependent optical selection rules make TMD monolayers and heterostructures ideal candidates for future valleytronics applications [2]. Confinement to a single layer and reduced dielectric screening result in a strong Coulomb interaction [3]. Excitons dominate the optical response and spin/valley properties [4], with clear differences from what expected from individual carriers. The non-linear optical response in layered materials and graphene is significant and can be modified by tuning the electronic properties [5]. This also allows external control of the non-linear optical generation [5]. I will outline recent progress on the exciton properties in monolayer TMDs [4]. I will discuss the spin-forbidden dark excitons [6] and related biexciton species [7] as examples to illustrate the unique spin and valley properties in monolayer TMDs. I will then discuss second and third harmonic generation from TMDs and Graphene [8], showing that the harmonic generation efficiency can be enhanced by over one order of magnitude by controlling the interplay between input fundamental frequency and Fermi energy.

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## Optical properties of all-inorganic perovskite nanocrystals

**Tom Gregorkiewicz**

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All-inorganic cesium lead halide perovskite nanocrystals (NCs,  $\text{CsPbX}_3$  NCs,  $X = \text{Cl, Br, I}$ ) attract much attention recently due to their outstanding optical properties. Here I will discuss our recent results concerning three important aspects of their micro-scopic characteristics: (i) an explicit demonstration of a relation between NC size and shape with their bandgap, and the effective coupling between proximal NCs; (ii) simultaneous formation of insulating  $\text{Cs}_4\text{PbBr}_6$  nanohexagons and  $\text{Cs}_4\text{PbBr}_6/\text{CsPbBr}_3$  hybrid nanospheres during the synthesis of  $\text{CsPbX}_3$  NCs; and (iii) spontaneous merging of drop-casted colloid at room conditions by seamless stitching of aligned NCs [1]. The latter process is accelerated by humidity and heat treatments, while arrested with electron beam irradiation. Further, I will present some detailed information on carrier dynamics in perovskite NCs, their water-resistant encapsulation, and on energy exchange within their ensembles obtained by using high-resolution induced absorption and emission spectroscopies. Finally, I will also discuss the most recent results concerning successful observation of efficient carrier multiplication in  $\text{CsPbI}_3$  NCs with bandgap energy around 1.8 eV [2].

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# Zero excess energy for carrier multiplication in van der Waals layered materials

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Carrier multiplication (CM), a photo-physical process to generate multiple electron-hole pairs by exploiting excess energy of free carriers, is explored for efficient photovoltaic conversion of photons from the blue solar band, predominantly wasted as heat in standard solar cells [1,2]. Current state-of-the-art approaches with nanomaterials have demonstrated the improved CM but are not satisfactory due to high energy loss and inherent difficulties with carrier extraction.

Here, we report efficient CM phenomena in van der Waals (vdW) multilayer that commences at the energy conservation limit and proceeds with high conversion efficiency [3]. A small threshold energy, as low as twice the bandgap, was achieved, marking an onset of quantum yield with enhanced carrier generation. Strong Coulomb interactions between electrons confined within vdW layers allow for rapid electron-electron scattering to prevail over electron-phonon scattering. In addition, the presence of electron pockets spread over momentum space could also contribute to the observed high CM efficiency. Combined with high conductivity and optimal bandgap, these superior CM characteristics identify vdW materials as an attractive candidate for third-generation solar cells.

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# Graphene films and membranes: fabrication and applications

**Hui-Ming Cheng**

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Graphene is a single-atom-thick sheet of hexagonally arranged, sp<sup>2</sup>-bonded carbon atoms that is not an integral part of a carbon material but is freely suspended or adhered on a foreign substrate, and has excellent properties, such as high mechanical strength and modulus, high thermal and electrical conductivities, very stable thermal and chemical stabilities, and unique electronic properties. Graphene films and membranes are expected to be used in various applications. Therefore, synthesis of graphene films and membranes in large area at reasonable cost is very important.

Basically, graphene films and membranes can be synthesized by CVD and assembly from chemically exfoliated graphene sheets. We developed an ambient pressure CVD to synthesize large and small size single crystal graphene grains, and their continuous films [1,2,3,4]. Moreover, we invented an electrochemical bubbling method to efficiently transfer these grains and films [2]. Large area and continuous graphene transparent conductive films are produced by an integrated R2R process of CVD and bubbling transfer. Very recently, we have developed a green electrochemical water oxidation exfoliation process of graphite to produce high-quality graphene oxide in large quantity and high yield [5], and invented a continuous centrifugal casting process to rapidly produce high-quality graphene membranes in large area and tunable thickness from chemically exfoliated graphene sheets [6]. These graphene films and membranes may have wide applications in many fields, from electronics to optoelectronics, from sensors to wearable devices, and from separation to water treatment [7,8]. However, great efforts are highly needed for the research, development, commercialization and market explorations of graphene films and membranes.

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## Atomically-precise graphene architectonics: 0D dots, 1D ribbons and 2D porous graphene

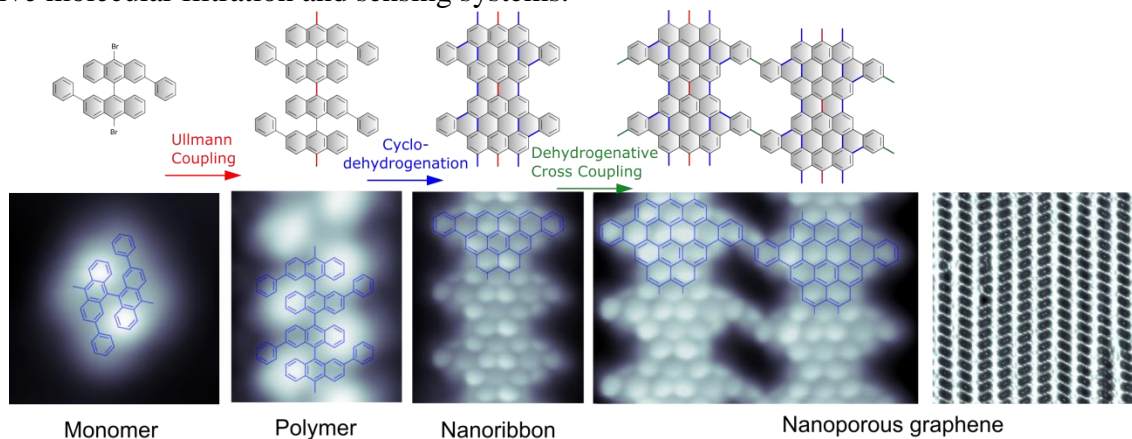
César Moreno

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On-surface reactions, via programmed interactions of molecular building blocks, has recently emerged as a promising route to synthesis atomically precise materials from the ‘bottom-up’. This approach ensures exquisite atomic-scale control of the structural and chemical functionalization, allowing to design a vast number of carbon-based nanoarchitectures not available by traditional solution chemistry nor with the ‘top-down’ methodologies. In particular, graphene nanoribbons (GNRs) with different structures can be synthesized with atomic precision and fine-tuned electronic band gap.

In this talk, I will describe the recent advances in the on-surface synthesis field. Then, I will discuss our recent results to synthesize 0D dots [1], atomically precise nanoporous graphene [2], graphene nanoribbons and their chemical functionalization and how to organize them into superlattices [3].

At the end of the day, this talk will demonstrate the full path to synthesize a semiconducting graphene material with a bandgap similar to that of silicon, its atomic-scale characterization, and its implementation in an electronic device. Further potential applications include in photonics and highly selective molecular filtration and sensing systems.



**Figure 1. STM images (bottom) and schematic representation (top) of the precursor, intermediates and final product of the hierarchical synthesis of nanoporous graphene.**

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# Room-temperature dilute magnetic semiconductor in V-doped monolayer WSe<sub>2</sub>

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Diluted magnetic semiconductors (DMSs) such as Mn-doped GaAs are attractive materials for gate-controlled spintronic devices but the low Currie temperature of the ferromagnetic order is far from room temperature, limiting for practical applications. In this talk, research challenges of DMSs will be reviewed. I will present our unambiguous observations of the long range ferromagnetic order occurring above room temperature in diluted V-doped mono layer WSe<sub>2</sub>. Magnetic hysteresis curves, micro magnetic domains and the well-defined structure of V-substituted W atoms are characterized by the vibrating sample magnetometer, magnetic force microscopy and high-resolution transmission electron microscopy, respectively. The possible mechanism of such high transition temperature in V-doped WSe<sub>2</sub> will be introduced by our band structure calculations based on density functional theory.

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# Spin generation from charge current, heat, and light

**Gyung-Min Choi**

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Manipulating magnetization by a spin current rather than a magnetic field is a fundamental issue in spintronics. To generate a spin current, some forms of energy is required. In this talk, I will review physical mechanisms for the spin generation from charge current, heat, and light, and my research for the spin generation will be shown accordingly. The mechanisms for the electrical spin generation are spin-filter effect, spin Hall effect, and Rashba effect [1-3]. The mechanisms for the thermal spin generation are spin-dependent Seebeck effect, spin Seebeck effect, and spin pumping effect [4-7]. The mechanisms for the optical spin generation are inverse Faraday effect, optical orientation, and photo-spin current [8-12].

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# Electronic correlations and pseudodoping in two-dimensional materials

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Two-Dimensional materials are in most cases not isolated but in direct contact to a substrate or part of vertical heterostructures. In this talk, we discuss how vertical coupling affects the electronic system of correlated two-dimensional materials. We firstly explain the effect of “pseudodoping”, i.e. apparent doping of metallic 2d materials without actual charge transfer, which occurs due to coupling to supporting substrates [1]. We then address the question of how electronic correlations and coupling to substrates can be exploited to switch 2d materials between conductive and insulating states. Examples of 2d Mott insulators [2] and impurities in 2d semiconductors will be considered.

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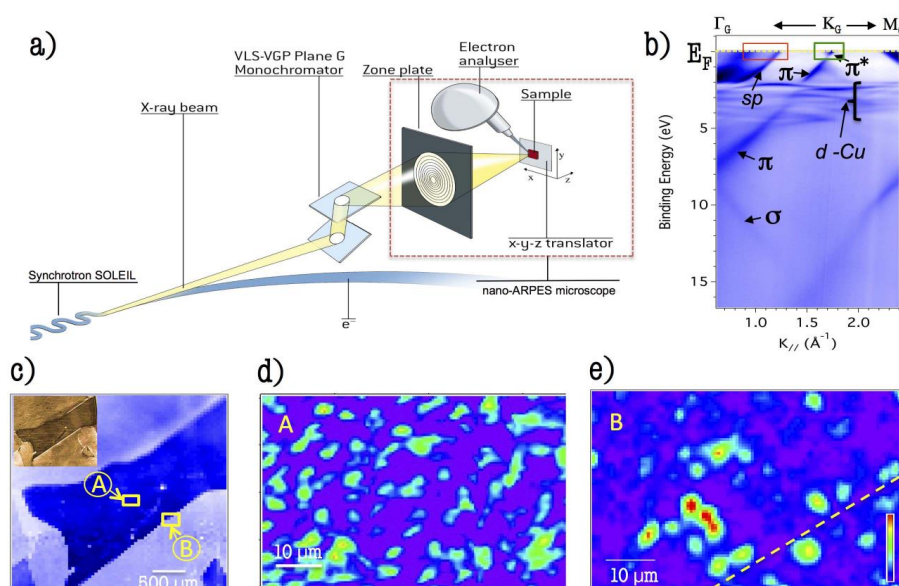
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# Electronic and chemical nano-imaging of 2D materials beyond graphene

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Recently, remarkable progress has been achieved in modern microscopies. However, even if they have attained exceptional lateral resolution, the problem of providing powerful spectroscopic characterization at the nano- and mesoscopic-scale still remains. This gap is particularly filled by an innovative and powerful technique named k-space nanoscope or NanoARPES (Nano Angle Resolved Photoelectron Spectroscopy). This cutting-edge nanoscope is able to determine the momentum and spatial resolved electronic structure, disclosing the implications of heterogeneities and confinement on the valence band electronic states typically present close to the Fermi level, see Fig. 1. The k-momentum space nanoscope can be effectively combined with chemical imaging based on core level scanning photoemission and X-ray absorption able to detect even very tiny different chemical environments.



**Figure 1.** Mixed real- and reciprocal-space images of a polycrystalline graphene film, grown on copper foils. (a) scheme of the nano-ARPES apparatus (b) ARPES data inside one of a large copper grain of the sample.

In the present talk, the more relevant innovations in the field of chemical and electronic imaging of 2D materials will be disclosed, highlighting the basic principles, associated instrumental and appealing scientific cases. In particular, nanoARPES findings describing the electronic band structure of mono-atomic exfoliated graphene on SiO<sub>2</sub> substrates, epitaxial and polycrystalline monolayer graphene films grown on copper and SiC [2] will be presented and Graphene/MoS<sub>2</sub> heterostructures. Electronic and chemical mapping with high energy, momentum and lateral resolution have provided relevant features like gap-size, doping, effective mass, Fermi velocity and electron-phonon coupling, among other properties for diverse 2D materials [3-6].

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## Manipulating light flow with 2D materials plasmons

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Recent years have observed a plethora of strong dipole type polaritonic excitations in 2D materials owing to the reduced screening. These polaritons can be sustained as electromagnetic modes at the interface between a positive and negative permittivity material. In the case of the plasmon-polaritons (e.g. in semi-metallic graphene), the negative permittivity is provided by the coherent oscillations of the free carriers. For exciton-polaritons (e.g. in semiconducting transition metal dichalcogenides, TMD) and phonon-polaritons (e.g. in diatomic hexagonal boron nitride, hBN), it is associated with their resonant optical absorption, resulting from a highly dispersive permittivity. These optical resonances can also result in a negative permittivity, albeit over a narrow spectral window.

In this talk, I will discuss our recent efforts in understanding plasmons behavior in 2D materials and using them to control the flow of light both in the far- and near-field. The general constitutive materials response of 2D materials, in conjunction with metasurface approaches, can potentially enable arbitrary control of phase, amplitude, polarization of light. The flow of light within the 2D materials can also exhibit rich transport behavior, such as hyperbolic rays, non-reciprocal chiral propagation, time reversal of waves and coupling of light spin to induce one-way propagation.

# Electronic structure and ultrafast dynamics of chalcogenide heterolayers

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The single-layer (SL) transition metal dichalcogenides (TMDs) display a diverse collection of intriguing electronic phenomena. These include single-particle and many-body effects encoded with spin- and valley-degrees of freedom [1,2]. By stacking SL TMDs of different compounds in bi-layer (BL) heterostructures an additional layer-degree of freedom becomes available, leading to further tunability of the optoelectronic properties [3].

I will present angle-resolved photoemission spectroscopy (ARPES) measurements incorporating micro- and nano-scale spatial resolution (microARPES and nanoARPES) performed on stacked layers of different TMD compounds ( $\text{WS}_2$ ,  $\text{MoS}_2$ ,  $\text{MoSe}_2$ ) with other two-dimensional materials such as graphene and hexagonal boron nitride (hBN). Our experiments reveal distinct superlattice effects associated with the type and twist-angle of adjacent materials in the stack, as well as the presence of one-dimensional scroll-like features around the edges of our stacks.

Using a single-domain crystal of two stacked layers of  $\text{MoS}_2$  (BL  $\text{MoS}_2$ ) we have explored the ultrafast response of a BL TMD to a polarization-tunable optical excitation in time-resolved ARPES (TR-ARPES) measurements. I will discuss the observation of a new type of layer-pseudospin effect emerging from quantum interference in the two TMD layers. This effect appears to completely dominate the ultrafast response of charge carriers near the K-point valleys of the BL TMD.

Finally, I will discuss the implications of our time- and spatially-resolved photoemission measurements for exploring non-equilibrium electronic and optical properties of low-dimensional materials *in situ*.

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## Toward single-crystal 2D materials on wafer scale

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Although large-area polycrystalline 2D materials have been realized by chemical vapor deposition, the structure defects such as grain boundary and point defects still degrades the unique material's properties. Here, we present the unique strategy of the self-collimation for the synthesis of single-crystal hexagonal boron nitride (SC-hBN) on a wafer scale [1]. The self-collimation between hBN grains is induced by the electrostatic interaction between boron and nitrogen atoms at peripheral hBN grains to eventually form the SC-hBN film on a liquid substrate. Furthermore, the synthesis of single-crystal graphene and transition metal dichalcogenides film on SC-hBN via epitaxial growth technique is demonstrated. The detailed growth mechanism and analysis will be presented.

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## **Discovery of new two-dimensional van der Waals materials: layered Zintl phases**

**Sung Wng Kim**

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The discovery of new families of two-dimensional (2D) van der Waals (vdW) layered materials has always attracted great attention to pursue beyond graphene. It has been challenging to artificially develop the van der Waals bonded layer structure that is constructed by the stacking of honeycomb atomic lattice composed of two elements as in hexagonal boron nitride. In this talk, a new class of 2D vdW materials, layered Zintl phases will be introduced. These new 2D layered Zintl phases can allow unlimited extent of 2D science in terms of the diversity of materials and their physical properties. A new class of 2D materials was developed from a 3D structured material that has (1) a multicomponent system, (2) primary atomic bonds in three-dimensionality, (3) thermodynamic and chemical stability, and (4) diversity in chemical compositions. Through the dimensional manipulation of crystal structure, we create an unprecedented 2D vdW zinc antimonide (2D-ZnSb), which is the layered Zintl phase with sp<sup>2</sup>-hybridized bonding characters in Zn-Sb honeycomb atomic layers. The vdW layered structure of 2D-ZnSb is evolved by selectively etching the lithium cations from the layered LiZnSb Zintl phase that is formulated by alloying the lithium atoms into sp<sup>3</sup>-hybridized bonded three-dimensional ZnSb (3D-ZnSb), demonstrating the bidimensional polymorphism of 3D- and 2D-ZnSb. The recent experimental and theoretical studies on diverse physical properties obtained in the new 2D materials will be discussed.

# ***Abstract***

## **Poster Session Monday**

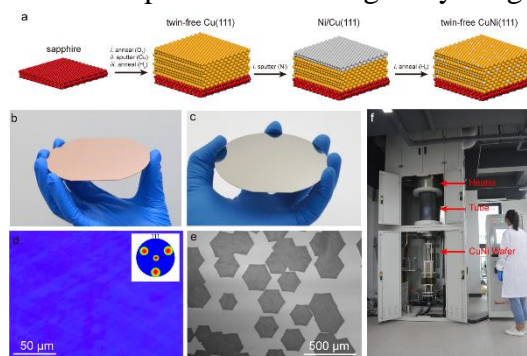
# Graphene as Electronic Materials: Controlled Growth of Single-Crystal Graphene Wafer

**Bing Deng**

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Similar to silicon (Si) wafers as the cornerstone of modern Si based electronics, single-crystal graphene wafers are vital components in future high-performance graphene electronics. Two approaches have been employed for single-crystal graphene growth by chemical vapor deposition (CVD), that is, the single-nucleation approach enabled by reducing the nucleation density, and the multi-nucleation approach featured with oriented graphene growth on an epitaxial substrate. Cu(111) is a substrate enabling epitaxial growth of graphene. We fabricated single-crystal Cu(111) thin films free of in-plane twinning on sapphire by magnetron sputtering and solid state recrystallization process. 4 inch single-crystal graphene was grown on the Cu(111) by APCVD.[1] The single-crystallinity was confirmed by multiscale characterization, including OM, SEM, Raman, LEED, and TEM. To improve the growth rate, single-crystal Cu<sub>90</sub>Ni<sub>10</sub>(111) thin films were fabricated. 4 inch single-crystal graphene was grown on the CuNi(111) within 10 min, 50 folds faster than that of Cu(111).[2] Single-crystal graphene grown on Cu(111) and CuNi(111) can be free of wrinkles, which further improved the electrical and mechanical properties of graphene.[3] One of the best benefits of graphene growth on the Metal(111) lies in the compatibility with wafer technology. A pilot-scale APCVD system is designed and built, and we are paving the way toward mass production of single-crystal graphene wafers.



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# Visualizing the Fast Growth of Large Single-Crystalline Graphene

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Chemical vapor deposition (CVD) technique has been demonstrated to be promising in growing large-area and high-quality graphene. However, the CVD-grown graphene is usually polycrystalline, which would degrade the electronic and mechanical properties. Consequently, to decrease the density of grain boundary, large single-crystalline graphene (LSCG) is synthesized via low supply of carbon source, which unfortunately exhibits low growth rate. Thus, fast growth of LSCG is an urging problem to realize the industrial growth of graphene film with high quality, which requires the in-depth understanding of the growth dynamics. Herein, we visualized the entire growth process of LSCG by using carbon isotopic pulse-labelling technique in conjunction with the Raman identification. The investigation of growth dynamics unveils the roles of carbon source in controllable growth of LSCG. By carefully tuning the carbon source supply, centimeter-sized graphene single crystals with high growth rate are realized.

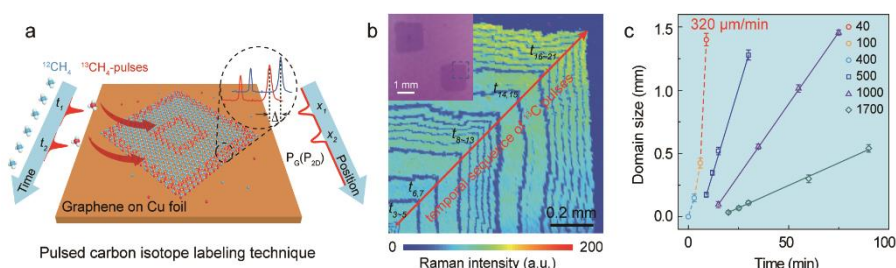


Figure: (a) schematic of visualizing fast growth of LSCG. (b) Optical image and Raman intensity maps of isotopic labeled LSCG. (c) Domain size as a function of growth time.

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# Fabricating high-efficiency silicon heterojunction solar cells with small-bundle single-wall carbon nanotubes

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Heterojunction solar cells based on single-wall carbon nanotubes (SCWNTs) and Si have been represented promising applications for photovoltaic devices, due to their simple device structures, low-temperature fabrication processes and promising performances [1]. SWCNT films with high optoelectrical properties are highly desired for improving photovoltaic conversion efficiencies and stability. In this work [2], we synthesized high quality and purity SWCNT films using a floating catalyst chemical vapor deposition method, which possess excellent optical and electrical properties (sheet resistance of  $\sim 200 \Omega \text{ sq}^{-1}$  with 90% transmittance at 550 nm). We constructed SWCNT/Si heterojunction solar cells by simply transferring the as-prepared SWCNT film onto the top surface of the Si substrate, and high power conversion efficiencies of 14.2% and 11.8% were achieved for devices with active areas of  $2.3 \text{ mm}^2$  and  $9.0 \text{ mm}^2$ , respectively. Furthermore, a high performance reproducibility and good stability were demonstrated, suggesting the superior potential of SWCNT/Si heterojunction for the next generation of photovoltaic devices.

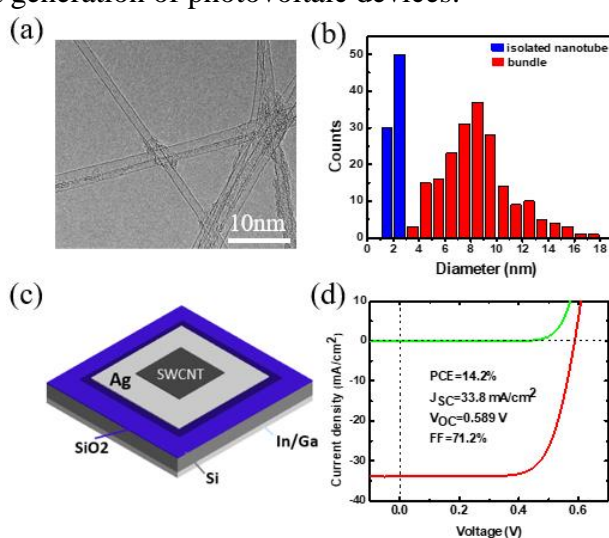


Fig.1 (a) TEM image of a SWCNT film; (b) Diameter distribution of the SWCNT filaments in the network measured from TEM images, showing a high fraction of isolated nanotubes and small bundles; (c) Schematic structure of a SWCNT/Si solar cell; (d) J-V curves of the best SWCNT/Si solar cell with a device area of  $\sim 2.3 \text{ mm}^2$ .

# Epitaxial Growth of 2D Metallic VSe<sub>2</sub> Single Crystals and their Heterostructures with Semiconducting MX<sub>2</sub>

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Two-dimensional (2D) metallic transition metal dichalcogenides (MTMDs) have recently emerged as a new class of materials for the engineering of novel electronic phases, 2D superconductors, magnets, as well as novel electronic applications. However, the mechanical exfoliation route is predominantly used to obtain such metallic 2D flakes, the batch production remains challenging. Herein, we report the van der Waals epitaxial growth of monocrystalline, 1T-phase, few-layer metallic VSe<sub>2</sub> nanosheets on an atomically flat mica substrate via a "one-step" chemical vapor deposition (CVD) method. The thickness of the VSe<sub>2</sub> nanosheets is precisely tuned from several nanometers to several tenths nanometers. More significantly, the 2D VSe<sub>2</sub> single crystals are found to present excellent metallic feature, as evidenced by an extra-high electrical conductivity of up to 106 S m<sup>-1</sup>, 1<sup>4</sup> orders of magnitude higher than that of various conductive 2D materials. The thickness-dependent CDW phase transitions are also examined through low-temperature transport measurements, which reveal that the synthesized 2D metallic 1T-VSe<sub>2</sub> nanosheets should serve as good research platforms for the detecting novel many-body states. The heterojunctions of VSe<sub>2</sub> and semiconducting TMDs also demonstrated in this work. The present results open a new path for the synthesis and property investigations of nanoscale-thickness 2D MTMDs crystals and metallic-semiconducting TMDs heterojunctions.

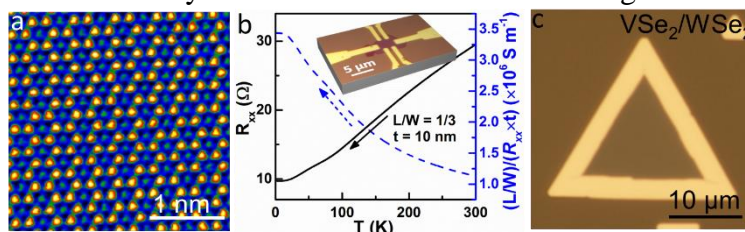


Figure 1. (a) Atomic-resolution HAADF-STEM image (filtered) of the VSe<sub>2</sub> nanosheet. (b) Temperature dependence of the resistivity (black line and arrow) and electrical conductivity (blue dashed line and arrow) for the VSe<sub>2</sub> device. (c) Optical image of as-grown VSe<sub>2</sub>/WSe<sub>2</sub> heterojunctions.

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# Directional distribution of Niobium atom interstitials in Nb<sub>2</sub>Se<sub>3</sub> compound alloy

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Nb<sub>2</sub>Se<sub>3</sub> has been known as one of quasi-one-dimensional conductors with chains of metal atoms that occupy a definite site in the structure [1]. This structure-related anisotropic property necessitates direct and simultaneous probing of atomic structure and the relevant chemistry for fundamental understanding of the material behaviour. To this end, we utilized scanning transmission electron microscopy (STEM) with energy dispersive X-ray spectroscopy (EDX) on the atomic level. Observing at different crystal zone axes, we revealed that two geometrically-distinguishable voids (V1 and V2) that are octahedrally-coordinated with Se atoms are distinguished with different volumes and bond distortions in the structure. Intriguingly, we found that Nb atoms preferentially occupy the V1 sites with the largest distorted volume and these Nb interstitials concurrently form a metal chain along the [010] orientation. Our finding strongly suggests that atomically-aligned Nb interstitial metal chains following the topologically-distinguished one-dimensional void network can contribute to the directional anisotropy in the electrical conduction and quasi-one-dimensional behaviour of Nb<sub>2</sub>Se<sub>3</sub> alloy. DFT calculations support that when Nb atoms occupy the V1 sites, the interstitial Nb atoms increase the charge density between inter-layer region of Nb<sub>2</sub>Se<sub>3</sub>, thus contributing to increasing DC conductivity.

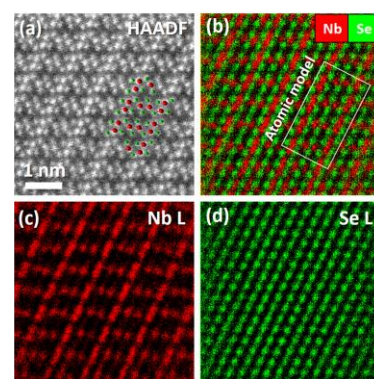


Figure 1. STEM EDX mapping of [010]-oriented Nb<sub>2</sub>Se<sub>3</sub> single crystal (red for Nb, green for Se). we

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# Mesoporous Graphene Frameworks and Its Application in VOCs Adsorption

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The volatile organic compounds (VOCs) are a series of organic compounds with high vapor pressures so that it'll be easy to vaporize and contaminate the air. The control of VOC emission is now a significant project with the increasing attention to environmental pollution. Methods like adsorption, condensation, filtration, and oxidation are often applied to lower the VOC content of the exhaust gases. It is commonly acknowledged that the most efficient way to treat gases with low concentration is adsorption. The Mesoporous Graphene Frameworks (MGF) is used as an adsorbent in this work. It shows a surprisingly high total adsorption capacity (AC) of 1289 mg VOCs/g MGF (Figure 1.a), which is much more than the adsorbents reported before (Figure 1.b).

Mesoporous Graphene Frameworks (MGF) is a kind of graphene with unique hexagonal 3-dimensional structure, high specific surface area (SSA, >2000 m<sup>2</sup>/g), and abundant mesopores. These characteristics enhance its ability to adsorb VOCs. In some recent works, we find a linear relationship between the SSA and AC for regular VOCs adsorbents, which is consistent with the adsorption model. However, the AC of our MGF is much more than expectations, which may indicate that the mesoporous structure is also essential in the VOCs adsorption process (Figure 1.b).

Because of the high AC, high efficiency, low pressure drop, easy recovery and recycling, MGF have potential applications as adsorbents in the future.

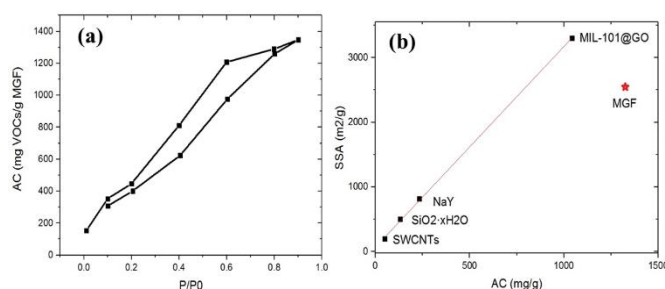


Figure 1: (a)The adsorption-desorption isotherms (b)Some adsorbents reported recently

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# Carbon fabric-based flexible supercapacitors with polydopamine-coated 3D carbon nanostructures

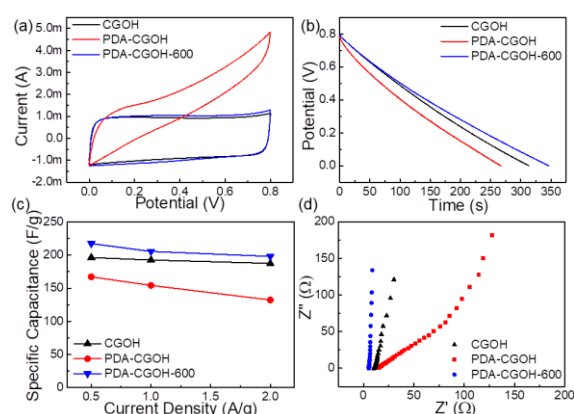
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Nowadays, wearable electronic technology, combination of portable electronics with wearable costume, is being widely researched, developed and applied in many fields of industry and human life. [1] A typical representation of energy storage devices are supercapacitors. The three-dimensional MWCNT/graphene hybrid hydrogel (CGOH) material was coated on carbon fiber fabric as electrodes and PVA/H<sub>2</sub>SO<sub>4</sub> was used as a solid electrolyte/separator layer in the flexible symmetric supercapacitor device. Polymer and heat treatment on the surface of CGOH was enhanced capacitance due to the formation and N-doping of graphitic layer.

The formation of polydopamine and graphitic layer on the surface of CGOH in the polymerization and carbonization process was decreased the BET surface area value of PDA-CGOH and PDA-CGOH-600 samples. In addition, the polydopamine layer is mainly reason of the change cyclic voltammetry (CV) curve shape due to the insulation property of polydopamine as shown in Fig. 1a. In comparison of PDA-CGOH-600 sample, the BET surface area is smaller than CGOH but the specific capacitance is enhanced by the formation of high conductive graphitic layer under without oxygen gas condition at high temperature as shown in Figure. [2] Moreover, the impedance test was investigated and the Nyquist plots were shown in Fig. 1d. In the high frequency region, the slope of PDA-CGOH-600 is higher than CGOH and PDA-CGOH to confirm the better supercapacitor characteristics.



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## Acknowledgement

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# Synthesis of Hierarchical Tree-like Few-layered MoS<sub>2</sub> Nanosheets Anchored on Vertically Aligned Carbon Nanotube Networks

**Jia Guo<sup>1,2</sup>, Yan Li<sup>\*1,2</sup>**

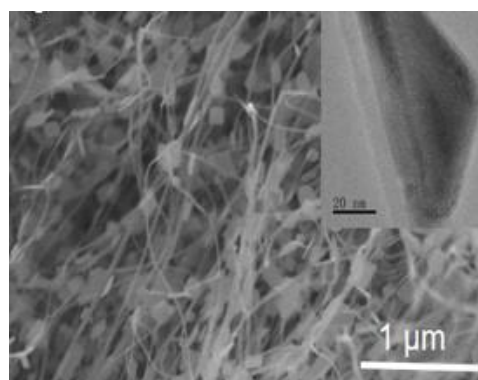
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Rational design and synthesis of hierarchical structures based on transition metal dichalcogenides (TMDs) and carbon nanotubes (CNT) have attracted increasing interests because of their promising applications in catalysis, etc. However, the construction of hierarchical structures with an interface at the edges of CNT still remains a great challenge.

Here, we report few-layered ultra-thin nanosheets of MoS<sub>2</sub> anchored on vertically aligned CNT nanohybrid networks over a large area (>1 cm<sup>2</sup>) are achieved by chemical vapor deposition technique. During the synthesis, with the optimized supply of precursor, highly uniform coverage along the longitudinal direction of MoS<sub>2</sub> nanosheets within CNT template which retains its original architecture is produced. In the resulting 3D architecture, the intimate contact between the edge of MoS<sub>2</sub> nanosheets and CNT can effectively avoid the aggregation and restacking of MoS<sub>2</sub> as well as remarkably increase effective specific surface area and obtain specific hierarchical porous nanostructures. The conductive matrix combines quasi-one-dimensional metallic nanotubes with two-dimensional semiconductive nanosheets which possesses subwavelength-structure inducing ultralow reflectivity property.



# Electrochemical Performance of poly sodium 4-styrenesulfonate intercalated thermally reduced graphite oxide paper for supercapacitors

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The electrochemical properties of poly sodium 4-styrenesulfonate intercalated thermally reduced graphite oxide (PSS-TRGO) for energy storage devices have been investigated and compared with 4-styrenesulfonate intercalated graphite oxide (PSS-GO) in a 1 M H<sub>2</sub>SO<sub>4</sub> electrolyte. The specific capacitance was improved from 200 F/g of PSS-GO to 250 F/g of PSS-TRGO at the scan rate of 50 mVs<sup>-1</sup>. The PSS-TRGO composite also demonstrate high energy density of 36 Whkg<sup>-1</sup> when its power density reaches to 611.3 Wkg<sup>-1</sup>, revealing the viability and potential for practical applications. The capacitance retention of PSS-TRGO was 97% after 1000 cycles, indicating high cyclic stability, and prominent performance as an electric double layer capacitor and even low resistance of the PSS-TRGO composite could be an excellent carbon based electrode for further energy storage devices.

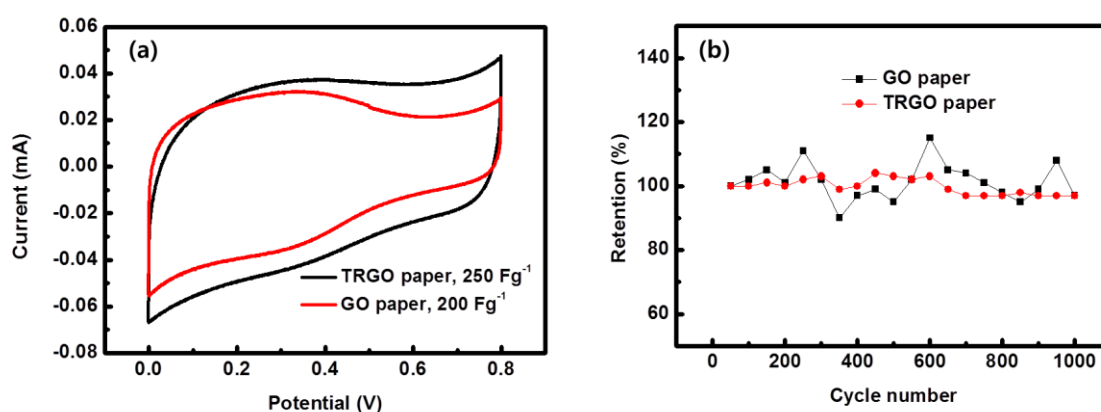


Figure (a) CV results of the composites (b) Capacitance retention of the composites.



# Functionalization of Thermally Reduced Graphite Oxide and Carbon Nanotubes by p-Sulfonatocalix[4]arene and Supramolecular Recognition of Tyrosine

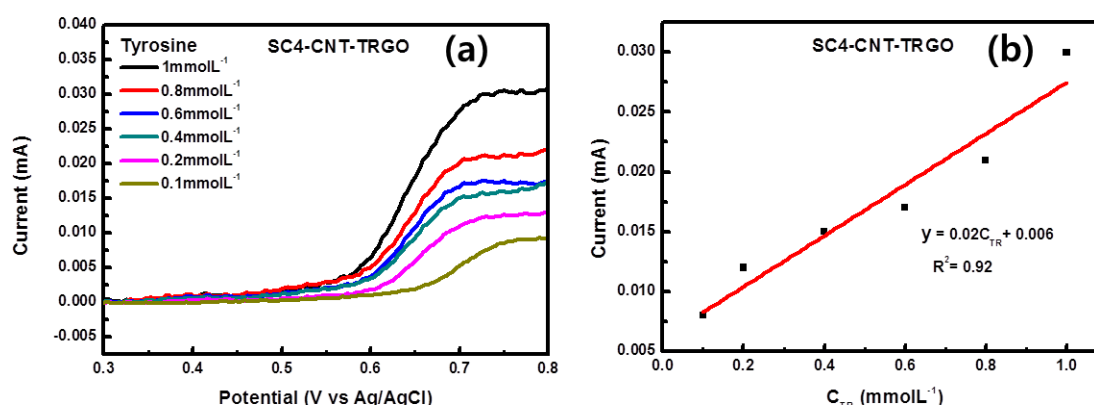
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p-Sulfonatocalix[4]arene-carbon nanotube (SC4-CNT), p-Sulfonatocalix[4]arene-thermally reduced graphite oxide (SC4-TRGO), p-Sulfonatocalix[4]arene-carbon nanotubes-thermally reduced graphite oxide (SC4-CNT-TRGO) are successfully synthesized by a simple chemical wet method. The obtained samples are characterized by using scanning electron microscopy, Fourier transform infrared spectroscopy, chronocoulometry, electron dispersive X-ray spectroscopy, cyclic voltammetry, and electrochemical impedance spectroscopy. The results confirmed that SC4 molecules are effectively loaded on the surface of CNT-TRGO composite compared to CNT and TRGO. The SC4-CNT-TRGO composite exhibits the highest supramolecular recognition of tyrosine and consequently excellent electrochemical response to the probe molecule compared to the other samples.

**Keywords:** reduced graphite oxide, carbon nanotube, p-Sulfonatocalix[4]arene, host-guest relationship, electrochemical detection.



**Figure 1.** (a) DPV response of SC4-CNT-TRGO at the different concentration and (b) it's calibration curve.

## Characterization of iron cerium oxide (FeCeOx) nanoparticles prepared by hydrothermal synthesis for hydrogen sulfide (H<sub>2</sub>S) removal application

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Materials for the reduction of hydrogen sulfide (H<sub>2</sub>S) have been extensively studied and have a number of achievements in the study of metal oxides. Notably, iron oxides in the form of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> as it meets the cost requirements and efficiency catalyst, but the catalysis effect of this material drops rapidly. Therefore, doping of other metal elements is expected to improve the catalytic activity and lifetime of Fe<sub>2</sub>O<sub>3</sub>. Among the doped heteroatoms, cerium (Ce) doped into Fe<sub>2</sub>O<sub>3</sub> exhibits a very high catalytic activity. In this paper, the catalyst of iron cerium oxide (FeCeOx) was synthesized by hydrothermal method with various temperature and annealing time. The FeCeOx nanoparticles were characterized by X-ray diffraction (XRD), Raman spectroscopy and Field emission scanning electron microscopy (FESEM), X-ray photoelectron spectroscopy (XPS). The results showed that the nanoparticles size of obtained FeCeOx was around 20-30 nm and size distribution was narrow.

**Keywords:** hydrothermal, FeCeOx, hydrogen sulfide.

**Acknowledgment:** The authors highly appreciate the financial support of Vietnam National University-Ho Chi Minh City for this research under the grant number C2017-32-04.

# Hierarchically-Structured Core-Shell Design of a Lithium Transition Metal Oxide Cathode Material for Excellent Electrochemical Performance

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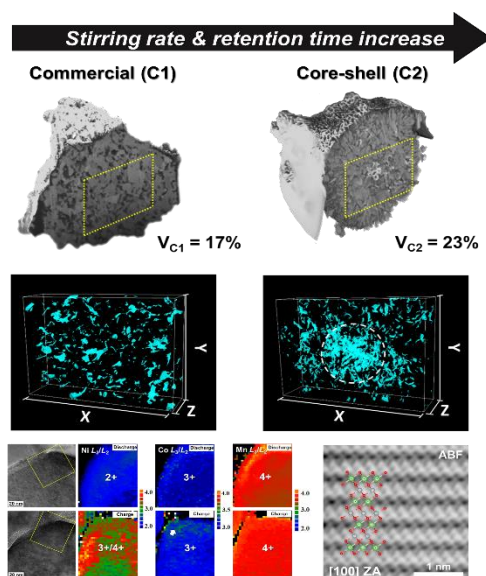
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Tailoring the geometric parameters of lithium-mixed transition metal oxide (LiTM) cathode materials is resource-efficient approach to enhancing the electrochemical performance of lithium ion batteries. In this study, we demonstrate that the overall electrochemical performance of active cathode materials can be significantly improved through the geometric design of LiTM cathode materials without needs of complex chemical modification or hetero structure engineering. Structurally optimized cathode material with a bimodal size distribution of primary particles inside the secondary particles is revealed to effectively reduce detrimental secondary reactions with electrolytes, thus resulting in high capacity and good durability: a 53.8% increase in capacity at a high discharge rates (10 C) as compared to commercial structures. The key concept of this approach is to maximize the beneficial effect of the controlled size of the primary particles, which allows facile and fast lithium ionization/extraction through a layered structure; Li diffusivity depends on the primary particle size having a huge influence on its migration path. Multimodal/multiscale microscopic characterizations based on electron tomography and scanning transmission electron microscopy, combined with electron energy loss spectroscopy (EELS) and energy-dispersive X-ray spectroscopy (EDS) from atomic to mesoscale levels, were employed to elucidate the structural origin of the enhanced battery performance. Our study paves a way for the resource-efficient microstructure design of LiTM cathode materials to maximize capacity and stability via simple adjustment of processing conditions, which is advantageous for mass production applications.



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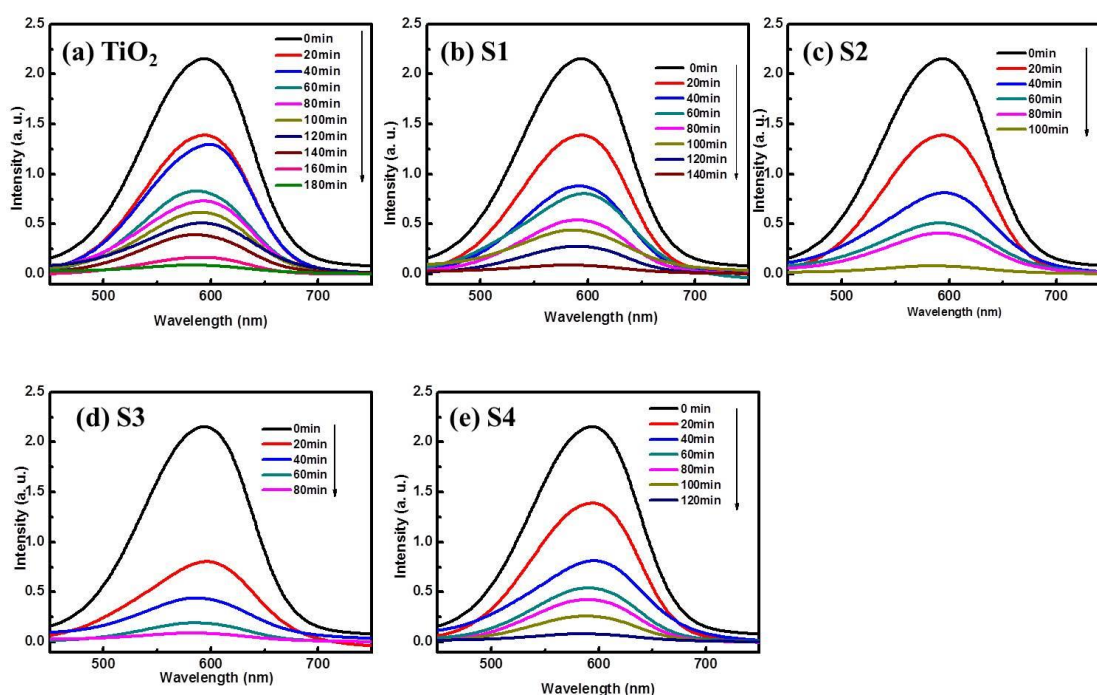
# Titanium Dioxide- Molybdenum Disulfide for Photocatalytic Degradation of Methylene Blue

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Photocatalytic degradation of methylene blue was carried out using titanium dioxide and molybdenum disulfide ( $\text{TiO}_2\text{-MoS}_2$ ) composite which was synthesized by using the sol-gel method. The composite had better performance in the photocatalytic degradation of methylene blue compared to pure  $\text{TiO}_2$  under irradiation of ultraviolet light. Weight ratio of  $\text{MoS}_2$  to CNT in the synthesis of the composite changed from 0.6 to 1.8, finding that the ratio of 1.4 provides the best photodegradation efficiency. The electrochemical results reveal that the introduction of  $\text{MoS}_2$  into  $\text{TiO}_2$  improves the lifetime of the photogenerated charge carriers, resulting in higher photocatalytic behavior in removing methylene blue.



**Figure 1:** UV-Vis spectra of the degradation of MB in the presence of the samples as a function of time interval of 20 min

# Quantification reliability of ADF-STEM imaging for vacancy concentration in 1L-TMDs

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Monolayer transition metal dichalcogenides (1L-TMDs) are promising two-dimensional semiconductors with direct bandgap, suitable for atomically thin nanophotonic device applications [1]. However, electronic property of the 1L-TMDs is significantly dependent on their chalcogen vacancies that are either intrinsically or extrinsically present. So, it is highly required to quantify the vacancy concentration in 1L-TMDs. Several exemplars for this have been recently reported with the help of atomic scale imaging capability of scanning transmission electron microscopy (STEM) [2, 3]. It is, however, unclear how reliable the method is because the quantification with statistical significance depends on the size of the image area, that is, the field-of-view of the STEM imaging, which is determined by the microscope magnification. In this study, we chose 1L-MoS<sub>2</sub> with intrinsic sulfur vacancies as a model sample and examined the effect of the field-of-view, statistical noise level, and the vacancy content on the precision of the defect quantification by systematic image simulations. Tracking the measurement precision with respect to those parameters, we determined the reliable range of imaging conditions for the defect quantification maintaining high accuracy at a level of  $\pm 0.1\%$ . Our approach offers an effective method to verify the measurement reliability of the atomic-scale STEM for the defect study on TMDs and provides more accurate information of the structural variation at an atomic scale to understand structure-property relationship of the materials.

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# Ligand exchange of colloidal WSe<sub>2</sub>: counter cation-dependent hydrogen evolution reaction (HER) study

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Hydrogen evolution reaction (HER) which involves the electrolysis of water molecules has been attracted as a clean synthesis of hydrogen, which is an alternative to steam methane reformer widely used in industry [1]. Among earth-abundant catalysts, promising candidates are transition-metal dichalcogenides (TMDs), which are two-dimensional (2D) layered materials; they can reach high current densities at low over-potentials [2]. Generally, these materials have been synthesized by vacuum-involving method like chemical vacuum deposition (CVD), while a colloidal synthesis has been less focused in spite of its scalable, less energy-intensive and cost-effective advantages [3]. The main reason is the existence of the surface ligands on the materials, resulting in the intrinsic limitation for a wide use as catalysts.

In this study, we demonstrate the effective ligand exchange of colloidal WSe<sub>2</sub> for a catalyst on HER. Up to now, it has been reported that the surface ligands block the catalytic reactions on the surface [3]; on the other hand, some other research groups have shown a lack of inhibition effects on certain ligands [4] or even an increase in the reactivity [5]. As a layered material, WSe<sub>2</sub> has a potential to intercalate small molecules between its layers. We found that after ligand exchange, this results in the incorporation of charge-balancing counter cations into the layers which increases the current density. In this presentation, we would like to introduce this effect on HER activity by electrochemical measurement, XRD, and XPS etc.

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# Intertwined Titanium Carbide MXene within 3D Tangled Polypyrrole Nanowires Matrix for Enhanced Supercapacitor Performances

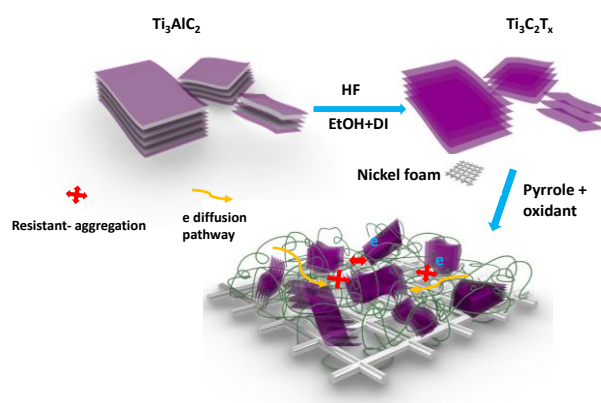
**Thi Anh Le<sup>1,2</sup> and Hyoyoung Lee<sup>\* 1, 2, 3,4</sup>**

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Exploring the rational design and synthesis of unique and robust architected electrodes for high capacitance, rate capability and stability of supercapacitors is crucial to the future of energy storage technology. Herein, an in-situ synthesis of multilayer-layered titanium carbide MXene tightly caging within three-dimension (3D) conducting tangled polypyrrole (PPy) nanowires network is proposed as an effective strategy to prevent the aggregation of MXene, profound enhancing the electrochemical performance of supercapacitor. Owing to the beneficial effects from ideal 3D interconnected porous and high electrical conductive, the obtained electrode exhibits the fast charges and ions transport kinetics as well as full active material usages. As expected, the 3D  $\text{Ti}_3\text{C}_2\text{T}_x$ @PPY NW exhibits a five-folds higher than that of pristine MXene in term of specific capacitance ( $610 \text{ F g}^{-1}$ ), good rate capability up to a current density of  $25 \text{ A g}^{-1}$  and excellent stability with 100% retention after 14000 cycles at  $4 \text{ A g}^{-1}$ , which outperforms the state-of-the-art of the known MXene-based supercapacitor. Our work provides a facile method to enhance the performance of MXene based-energy storage devices.



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T.A Le et al, Chem.Eur.J.10.1002/chem.201804291.

## Fabrication and characterizations of MoS<sub>2</sub>/Au nanogratings

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Growing research attention has been paid to how surface plasmons (SPs) can influence the optical properties of transition metal dichalcogenide (TMD) layers. Numerous works have been reported regarding the exciton-SP coupling [1]. The resonance wavelength of SP can be controlled by the size, shape, and dielectric function of the metal nanostructures, as well as the dielectric environment [2]. In this work, a few layers of MoS<sub>2</sub>, a representative 2D TMD semiconductor with visible-light-range band gap energy, were transferred on Au nanogratings and their physical characteristics were studied. In the MoS<sub>2</sub>/Au nanograting samples, the influences of strain [3] and interface dipoles at the Au/MoS<sub>2</sub> interface [4] also should be considered. To clearly understand the roles of the SP excitation, two kinds of the Au gratings were prepared: Au stripe arrays on bare SiO<sub>2</sub>/Si (type I) and Au-coated SiO<sub>2</sub>/Si (type II) substrates. Finite-difference time-domain simulation showed clear reflectivity dip as a signature of propagating SP polariton excitation only in the type II Au gratings under TM-mode light illumination. The work function of the MoS<sub>2</sub> layers were measured by Kelvin probe force microscopy in dark and under the TM/TE-mode light illumination. We could propose band diagrams of the MoS<sub>2</sub> flakes on the Au nanograting structures to explain all the experimental results. This study can help us to understand and control the physical characteristics of the TMD/metal nanostructures.

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# Toward ultraclean 2D heterostructure interfaces: h-BN as a novel tool to visualize organic residues

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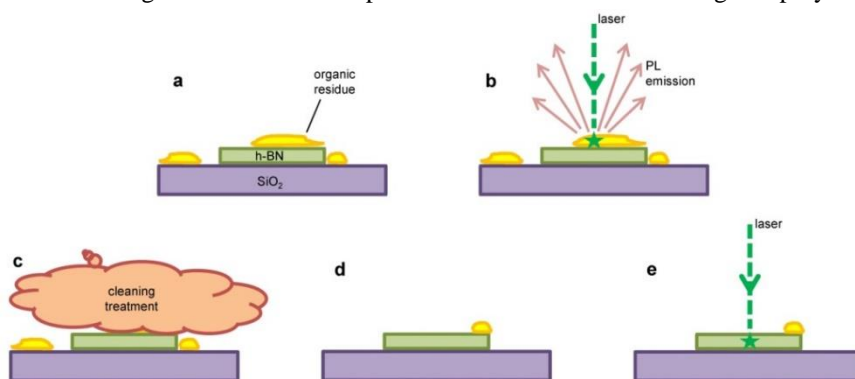
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The search for novel physics in 2D Van-der-Waals heterostructures is greatly dependent on the availability of high-quality samples. For example, previously, 2D sample quality was often limited by the SiO<sub>2</sub> substrate, which is rough and contains a high density of charged impurities. This limitation can be overcome by using h-BN as a substrate: h-BN is ultraflat and free from charged impurities, typically resulting in dramatically enhanced sample quality, and this approach has enjoyed enormous popularity in recent years. Nonetheless, frequently extrinsic factors continue to limit the quality of 2D heterostructures, and one of these factors is the presence of organic processing residues, such as adhesives from mechanical exfoliation or residues from transfer and lithography steps, which can be left on sample surfaces and trapped at interfaces.

A number of approaches have been developed to reduce and remove such organic polymer residues, but many techniques suffer from drawbacks, and their applicability tends to be highly specific to the sample material. For example, acetone cleaning approaches most often lead to incomplete residue removal only; recipes involving heating the sample in vacuum or in inert gas, instead of evaporating organic residues often spread the residues across the sample; and oxidative heating methods are incompatible with reactive 2D materials such as black phosphorus. Thus, development of new 2D material cleaning recipes that address these shortcomings is highly desirable.

A key obstacle in the development of new cleaning recipes is the difficulty in detecting organic residues, which complicates the evaluation of cleaning efficacy; organic polymer films of nanometer thickness are typically transparent and liquid-like, and common sample characterization methods such as optical microscopy, atomic force microscopy, or Raman spectroscopy are not suitable to detect their presence. To overcome this obstacle, we study the intense luminescence of 2D hexagonal boron nitride (h-BN) in the presence of organic residue. We exploit the observation that thin organic polymer films deposited on h-BN lead to very bright photoluminescence [1], enabling us to visualize even minute amounts of organic residue. This phenomenon is unique in its ability to visualize minute amounts of organic contaminants that are invisible by other means, and I plan to exploit it as a tool to develop efficient processing and cleaning methods for the fabrication of ultraclean 2D heterostructure interfaces. Our approach involves the preparation of exfoliated h-BN samples, which we deliberately contaminate with the target organic polymer of interest, such as adhesive residue. For a given candidate cleaning method, we then acquire photoluminescence maps before and after the cleaning step, enabling a clear assessment of the recipe's effectiveness.



Separately, h-BN has recently been reported as a host to room temperature quantum emitters a phenomenon previously observed in wide-bandgap 3D semiconductors such as diamond and nanocrystal quantum dots. In this work, I study the room temperature emission properties of h-BN flakes under green laser excitation (532 nm). Using photoluminescence spectroscopy, I observe emission from isolated defect sites and characterize their spatial distribution and temporal evolution in detail, with the goal to understand the physical mechanism of this phenomenon

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# Carbon-based Asymmetric Capacitor for High-Performance Energy Storage Devices

**Doyoung Kim<sup>1,3,†</sup>, Keunsik Lee<sup>1,2,†</sup>, and Hyoyoung Lee<sup>\*1,2,3,4</sup>**

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Carbon-based materials are widely used in energy storage research, as attractive materials with high conductivity, low cost, and high availability.[1] However, a relatively low performance (e.g., energy and power densities) compared with metal oxides is an obstacle to use for commercial applications. Researchers have achieved a high performance capacitors with the use of pseudocapacitance of metal oxides depending on redox reactions.[2-3] But the drawbacks are a low conductivity and low stability of the metal oxides. On the other hand, non-faradaic capacitance due to accumulated charges in carbon-based electrodes resulted in a high conductivity and high stability, even though this exhibit a relatively lower performance than metal oxide pseudocapacitance capacitors. Herein, we report on high-performance metal oxide-free asymmetric capacitors (ASCs) using n-type and p-type graphene films which are doped by nitrogen and boron atoms, respectively, exhibiting high energy and power densities with excellent stability. The enhanced performances of the ASCs arises from the synergistic effect of the non-faradaic capacitance and pseudocapacitance, which are confirmed with new analysis using cyclic voltammetry and electrochemical impedance spectroscopy for an pseudocapacitance effect of intercalation/deintercalation and galvanostatic charge-discharge profiles for and non-faradaic capacitance. The new ASC shows the high energy density of 77.41 Wh kg<sup>-1</sup> in 3.0 V of the operating potential window with the excellent retention stability of ~87% after 10,000 cycles. The carbon-based asymmetric capacitor of semiconducting graphene electrodes can offer the promise of exploiting both non-faradaic capacitance and intercalation/deintercalation pseudocapacitance to obtain a high-performance energy storage device.

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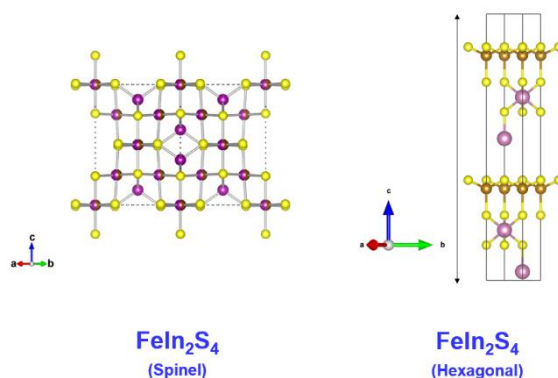
# Colloidal Synthesis of Hexagonal FeIn<sub>2</sub>S<sub>4</sub> and its Layer Dependent Band Structures

**Hyunjung Kim<sup>1,4</sup> and Hyoyoung Lee<sup>\* 1, 2, 3,,4</sup>**

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Here, as a new candidates of two dimensionally confined nanomaterials, a ternary metal chalcogenides, hexagonal FeIn<sub>2</sub>S<sub>4</sub> (h-FIS) were newly introduced with layer dependent characteristic. Similar to the exotic electrical, chemical and physical properties of conventional two dimensionally confined materials,[1] the as synthesized hexagonal FeIn<sub>2</sub>S<sub>4</sub> also exhibits different energy band gap and states, which is highly dependent on the number of layers. In the synthetic point of view, different number of layers could be obtained by controlling the sulfur radical dissociation rate, showing significantly similar growth tendency of two dimensional layered structure formation in colloidal synthesis. [2] Different crystal structure between hexagonal and cubic FeIn<sub>2</sub>S<sub>4</sub> was compared with X-ray diffraction (XRD) data and raman scattering. In addition, UV-vis spectroscopy and cyclic voltammetry measurement were conducted on h-FIS with different number of layers to obtain the optical bandgap and redox potentials, respectively. Finally, each conduction and valence band was investigated based on the redox potentials and correlated with the optical bandgap of h-FIS. This study will contribute to exploring unveiled characteristics of ternary metal chalcogenides and new low dimensionally confined materials.



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# Non-enzymatic glucose sensor based on CuO nanoparticles modified screen-printed carbon ink electrode

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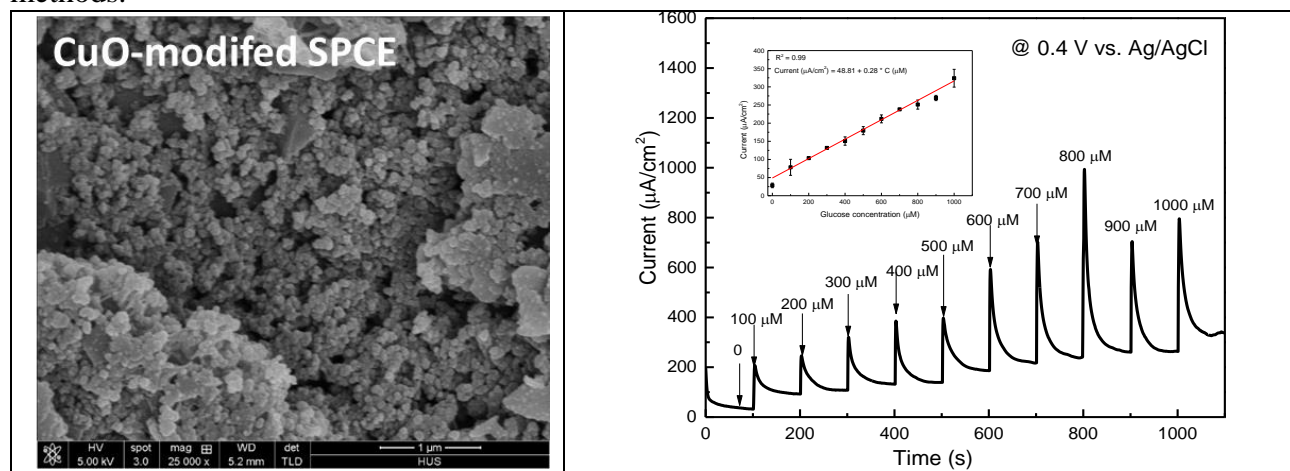
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In Vietnam, the prevalence of diabetes is growing at alarming rates and has almost doubled within the past 10 years. Monitoring glucose levels in blood is an effective method to diagnose of diabetes, and to optimize patient treatment strategies. Thus, many efforts have been devoted to develop a highly sensitive and selective glucose sensor. The non-enzymatic amperometric glucose sensors have high repeatability and stability compared to enzymatic sensors. In addition, they are easy to become commercial products which have practical significance in clinical diagnosis.

A widely investigated material for using as a non-enzymatic glucose sensor is CuO due to nontoxic nature and its outstanding redox behavior as well as efficient catalyst for oxidative. The corresponding nonenzymatic response process to glucose detection is following steps: First, the  $\text{Cu}^{+2}$  of CuO transforms to  $\text{Cu}^{+3}$  in form of  $\text{CuO}(\text{OH})$  at the optimal potential in NaOH solution, resulting in releasing one electron. Then,  $\text{Cu}^{+3}$  obtains an electron and acts as an electron delivery system under the presence of glucose. Thus, electrons are transferred from glucose to the electrode that leads to the increasing of the current.

In this work, screen-printed carbon ink electrode (SPCE) was used as a transducer for non-enzymatic glucose sensor. The CuO nanoparticles were synthesized on the surface of working electrode by using the cyclic voltammetry (CVs) method. Glucose sensing performance was measured in 100 mM NaOH at constant potential of 0.4 V vs. Ag/AgCl. Figure 1 shows the SEM image of CuO/SPCE and transient response to different glucose concentrations. The results show that the current increases with increasing of glucose concentration. The sensitivity of the sensor was  $0.3 \mu\text{A} \cdot \text{cm}^{-2} / \mu\text{M}$ . The fabricated sensor was applied to detect glucose in blood samples and shows comparable to clinical diagnosis methods.



**Figure 1.** a) SEM image of CuO-modified SPCE and b) transient response to different glucose concentrations of non-enzymatic biosensor based on CuO nanoparticles decorated on SPCE.

# Ultralight and Flexible Sodium Titanate Nanowire Aerogel with Superior Sodium Storage

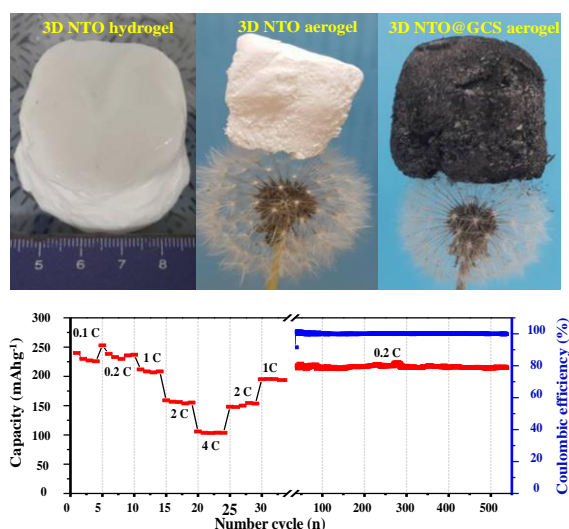
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An ultralight, conductive, and flexible 3D assembly of a metal oxide nanowire aerogel as an electrode for energy storage devices without additives and the typically inconvenient flexible supported-substrate remains a challenge. Herein, we report a new 3D highly-ordered layer-by-layer stacking sodium titanate@reduced graphene oxide core-shell (NTO@GCS) nanowire aerogel that has an ultra-high aspect ratio with a diameter of 30-50 nm and typical length up to 100  $\mu\text{m}$  for a new class of convenient sodium-ion battery (SIB) anode. The formation mechanism of the unique 3D NTO nanowire aerogel, the precursor of the NTO@GCS aerogel, was carefully proposed, demonstrating that the key challenge for this synthesis strategy was to form a stable and homogeneous ultrafine NTO nanotube gel suspension. In addition, for high performance sodium-ion storage, reduced graphene oxides (rGOs) were introduced into the NTO aerogel backbone. The critical role of the graphene structure between the NTO nanowires and rGO sheets in Na<sup>+</sup> storage was systematically investigated. Compared to the 3D pristine NTO aerogel and 3D NTO nanowires on graphene sheet paper, the 3D interconnected NTO-GCS aerogel electrode facilitated ion electrolyte transportation, resulting in remarkably enhanced Na<sup>+</sup> storage with a reversible capacity of 240 mAh g<sup>-1</sup> at 0.2 C and durable cycling stability after 4,900 cycles at a rate of 2 and 4 C with nearly 100% Coulombic efficiency.



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Ngoc Quang Tran, Thi Anh Le, Hyoyoung Lee “An ultralight and flexible sodium titanate nanowire aerogel with superior sodium storage” J. Mater. Chem. A. 2018, 6, 17495-17502.

## Fabrication of Hydrogen Gas Sensor Based on SnO<sub>2</sub>/Pt Thin Film on Kapton Substrate

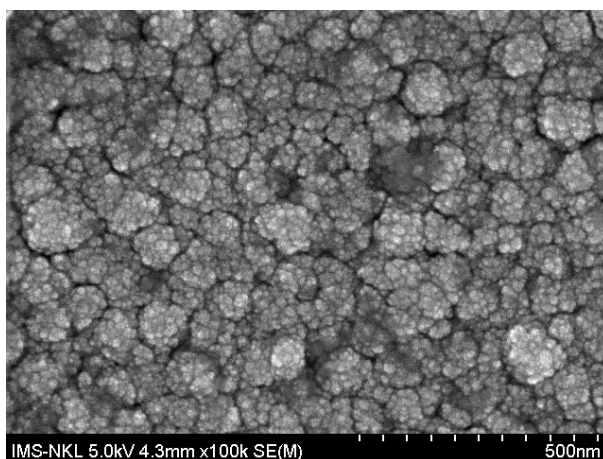
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We report gas sensing properties of SnO<sub>2</sub>/Pt thin film on flexible substrate prepared by sputtering for low temperature hydrogen detection. The sensor electrodes with Pt/Cr on polyimide substrate were fabricated by photolithography in combination with sputtering method. Then the sensing layers of SnO<sub>2</sub> and Pt were deposited onto the electrodes. Before studying, the sensor was annealed to 350°C in different time to stabilize the thin film contacts and materials. The morphology of sensing layer was studied by scanning electron microscopy, whereas hydrogen sensing properties were measured at different temperature and gas concentration. The fabricated sensor presented a high gas response to 25 ppm H<sub>2</sub> at working temperature of 100°C with the response and recovery times of hundreds seconds. The stability of the sensor after substrate bending was also investigated. The obtained results indicated the successful fabrication of sensitive hydrogen sensor on flexible substrate for low temperature application.

Keywords: SnO<sub>2</sub>/Pt thin film; flexible sensors; hydrogen gas sensor.





# Engineering on Ni-Co-S Bifunctional Electrocatalyst for Water-splitting

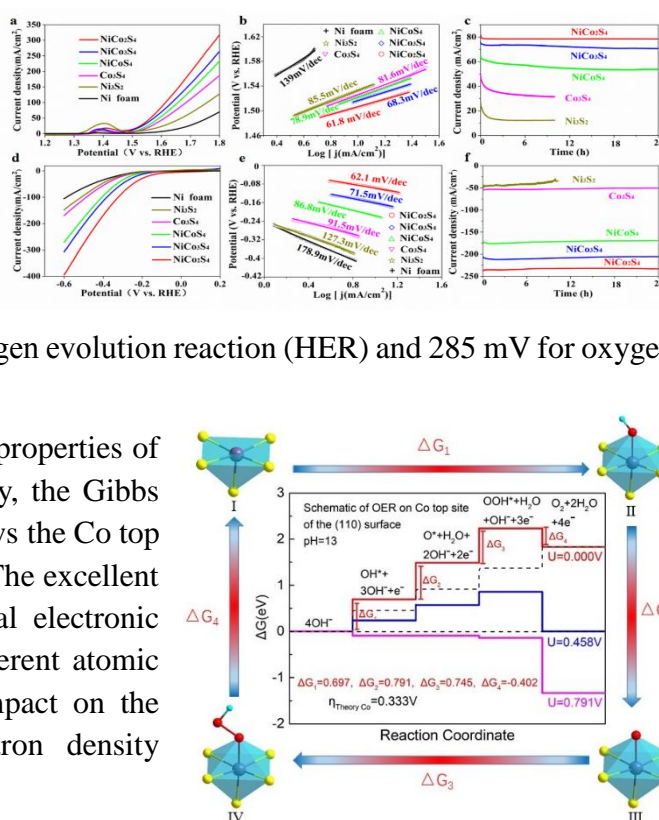
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Ni-Co-S is a technologically important electrode material that has recently achieved remarkable performance in catalysis. Herein,  $\text{Ni}_x\text{Co}_y\text{S}_4$  bifunctional catalysts with tunable stoichiometry was synthesized on Ni foams. The electronic structure engineering contributed to the significantly elevated electrocatalytical performance. As a result, overpotentials  $\eta_{10}$  of 97 mV (vs.RHE) for hydrogen evolution reaction (HER) and 285 mV for oxygen evolution reaction (OER) in 1M KOH solution.

At the same time, we study the electrocatalytic properties of the NiCo<sub>2</sub>S<sub>4</sub> by using density functional theory, the Gibbs free energy changes of different active sites shows the Co top site of the (011) surface is the most active site. The excellent catalytic activities are attributed to the optimal electronic structure of catalyst surface, we found the different atomic ratios between Ni and Co have significant impact on the electronic structure by calculating the electron density difference of Ni<sub>x</sub>Co<sub>y</sub>S<sub>4</sub>[1, 2, 3].



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# Theoretical Insights into the Size-Dependent Ru Clusters on N-doped Graphene for Electrocatalytic Hydrogen Evolution and Oxygen Reduction Reactions

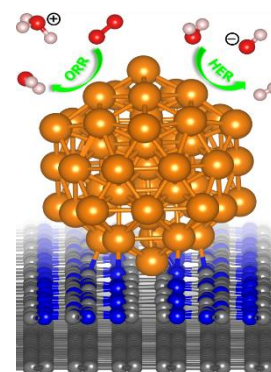
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The variant size of metal clusters demonstrates markedly different catalytic behaviors in the heterogeneous catalysis. However, the molecular-level synergistic influence of the metal cluster size supported on various substrates as well as its utmost utilization on the catalytic activities has till been limited. Here, we performed density functional theory (DFT) calculations under experimental conditions to elucidate the size-dependent activity of electrocatalytic hydrogen evolution (HER) and oxygen reduction reactions (ORR) over Ru clusters on the N-doped graphene (g-CN). Four size-selected Rux clusters ( $x = 4, 6, 13, 55$ ) on g-CN (Rux@g-CN) were demonstrated in terms of the stability, electronic properties, both HER and ORR activities, and their enhanced catalytic efficiency as placing Rux@g-CN on graphene (Rux@(g-CN/G)). Our result shows that large Ru cluster size, in Ru-55 particular, on both g-CN and (g-CN/G) seems to be optimal for HER in basic and ORR in acidic media. Furthermore, we provide the detailed information of the favorable HER-ORR reaction pathways over each cluster size supported on g-CN and g-CN/G, which helps to get the fundamental understanding of the size effects on the catalytic performance.





# Molecularly ultrathin sheets of Fe-graphene on nickel foam supported NiCo<sub>2</sub>O<sub>4</sub> microrod arrays as a highly efficient bifunctional electrocatalyst for oxygen and hydrogen evolution reaction

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Electrochemical water splitting has a significant role in sustainable energy technologies like fuel cells.[1] Catalysts play a worthwhile role in both anodic (Oxygen evolution reaction/OER) and cathodic (Hydrogen evolution reaction/HER) reactions. Engineering fine micro/nanostructure with subtle morphologies represents an effective strategy to enhance the activity of the resultant catalyst towards OER and HER through exposing abundant electrochemically active sites. To reduce fabrication cost of water electrolyzer, it is highly desirable to explore a bifunctional electrocatalyst with high activity toward both OER and HER in the same electrolyte. [2] In this report, we developed a bifunctional electrocatalyst for efficient water splitting by developing ultrathin Fe and graphene layer on the surface of NiCo<sub>2</sub>O<sub>4</sub> that is vertically aligned micro rods on nickel foam substrate using two-step process. In first step, NiCo<sub>2</sub>O<sub>4</sub> micro rods array deposited on NF by assistance of diethylenetriamine and metal salt using hydrothermal followed by air annealing method. In the next step, thin sheets of graphene and Fe electrochemically deposited, resulting material named as Fe-graphene@NiCo<sub>2</sub>O<sub>4</sub>@NF. The prepared composite electrode provided the benchmark current density of 10 mA cm<sup>-2</sup> for HER and OER, at a low overpotential of 155 mV and 214 mV, respectively. The long-lasting stability of Fe-graphene@NiCo<sub>2</sub>O<sub>4</sub>@NF electrode along with its exceptional catalytic activity makes it as a promising alternative to replace the precious metal catalyst used in commercial water electrolyzer.

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# Intercalates-Assisted Electrochemical Transfer of Monolayer WS<sub>2</sub> Film on Gold substrate

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Yang<sup>1,\*</sup>, and Ki Kang Kim<sup>2,\*</sup>**

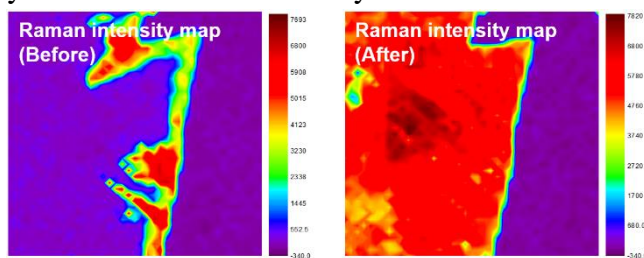
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Gold has been proposed as a promising substrate for the growth of semiconducting transition metal dichalcogenides (TMDs) [1-3]. However, the strong interaction between TMDs and the gold substrate hinders the delamination of TMDs layer from the gold substrate during electrochemical transfer [3]. Herein, we systematically investigate the intercalation of sulfur-involved gas molecules, which easily diffuse between the gold surface and the as-grown TMDs (eg. WS<sub>2</sub>). By way of intercalating gaseous molecules between the gold substrate and as-grown WS<sub>2</sub>, the interaction between the gold substrate and WS<sub>2</sub> is significantly weakened, resulting in enabling electrochemical transfer process. The reducing the interaction between gold and WS<sub>2</sub> is confirmed via scanning electron microscopy, Raman spectroscopy, kelvin probe force microscopy, revealing that the temperature and duration for intercalation are crucial factor for the successful delamination of WS<sub>2</sub> from gold. Eventually, the centimeter-scaled monolayer WS<sub>2</sub> film is successfully transferred onto a target substrate.



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# Graphdiyne Nanowall for Enhanced Photoelectrochemical Performance of Si Heterojunction Photoanode

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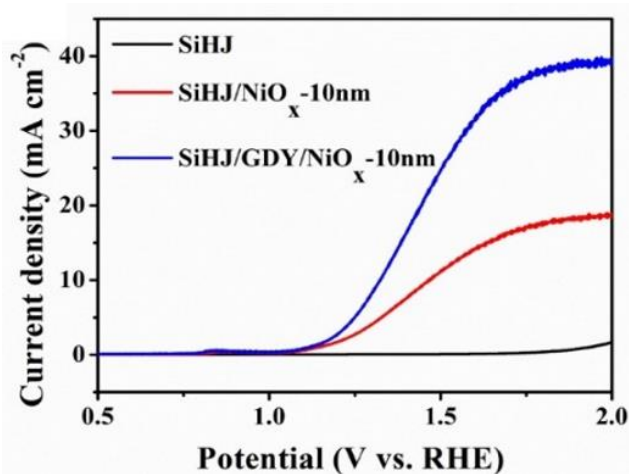
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Silicon is a promising photoelectrode material, whose commercial application is impeded by its sluggish oxygen evolution reaction (OER) dynamics in electrolytes [1, 2]. Graphdiyne (GDY), a new member of 2D carbon material family [3], was introduced into a Si heterojunction (SiHJ) based photoelectrochemical water splitting cell (PEC). Polarization curves measurement showed that the plateau photocurrent density of SiHJ/GDY/NiO<sub>x</sub>-10 nm with optimized NiO<sub>x</sub> film thickness was twice higher than that of SiHJ/NiO<sub>x</sub>-10 nm, demonstrating the catalytic function of GDY itself as well as the synergistic effect between GDY and NiO<sub>x</sub>. The results verified that GDY is a promising photoelectrode material candidate to realize highly efficient PEC performance, and pave a novel pathway to further improve Si based PEC system.

In this study, for the first time, we successfully introduced GDY into the Si-based photoelectrochemical system for water splitting. The GDY nanowalls and subsequent magnetron sputtered NiO<sub>x</sub> nanoparticles were employed on the top of SiHJ (Si heterojunction) for photoinduced hole transfer facilitation and oxygen evolution catalysis. NiO<sub>x</sub> and GDY have been characterized to be respectively capable to catalyze water oxidation as previously reported [4]. Meanwhile, the chemical bonds between GDY and NiO<sub>x</sub> led to the synergistic effect, which contributed to the further catalytic enhancement only with proper NiO<sub>x</sub> thickness. As can be seen in the right figure, the saturated photocurrent density reaching up to 39.1 mA cm<sup>-2</sup> indicated the superiorities of GDY introduction to Si based PEC system, and again verified the universal significance of GDY in solar energy harvesting and other related energy conversion applications.



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# Wafer-scale van der Waals heterostructures with ultraclean interfaces via the aid of viscoelastic polymer

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Two-dimensional (2D) van der Waals (vdW) heterostructures exhibit novel physical and chemical properties, allowing the development of unprecedented electronic, optical, and electrochemical devices. However, the construction of wafer-scale vdW heterostructures for practical applications is still limited due to the lack of well-established growth and transfer techniques. Herein, we report a method for the fabrication of wafer-scale 2D vdW heterostructures with ultraclean interface between layers via the aid of freestanding viscoelastic polymer support layer (VEPSL). The low glass transition temperature ( $T_g$ ) and viscoelastic nature of VEPSL ensures absolute conformal contact between 2D layers, enabling the easy pick-up of layers and attaching to other 2D layers. This eventually leads to the construction of random sequence 2D vdW heterostructures such as molybdenum disulfide/tungsten disulfide/molybdenum diselenide/tungsten diselenide/hexagonal boron nitride. Furthermore, VEPSL allows the conformal transfer of 2D vdW heterostructures onto arbitrary substrates, irrespective of surface roughness. To demonstrate the significance of the ultraclean interface, fabricated molybdenum disulfide/graphene heterostructure employed as an electrocatalyst, yielded excellent results of 73.1 mV·dec<sup>-1</sup> for Tafel slope and 0.12 k $\Omega$  of charge transfer resistance, which are almost twice lower than that of impurity-trapped heterostructure.

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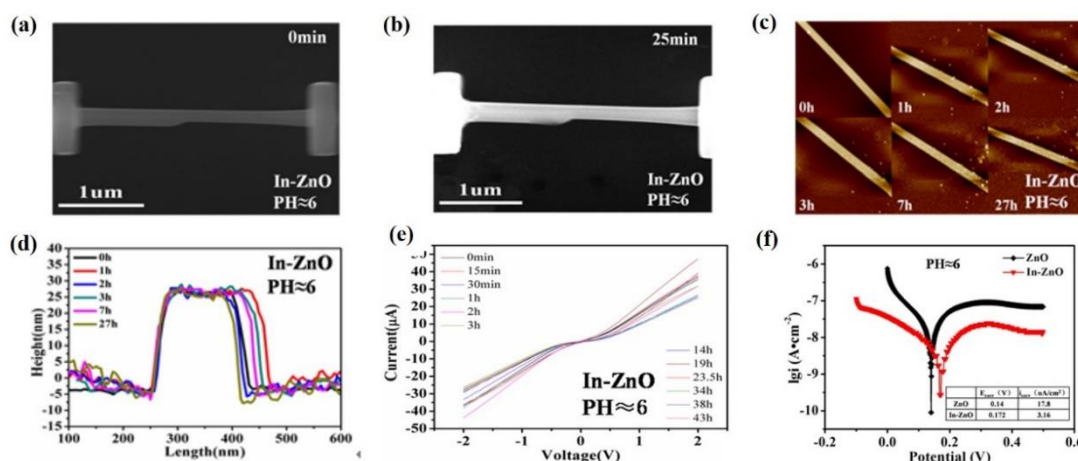
# Influence of Indium doping on dissolving behavior and stability of quasi-2D ZnO nanobelts in solution

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**Abstract:** Because of its direct wide band-gap ( $E_g = 3.37$  eV at room temperature), large exciton binding energy (60 meV), and remarkable electromechanical properties, ZnO can be used as the basic structural units of the field effect transistors (FETs), sensors, lasers, nanogenerators and photovoltaic (PV) applications [1,2]. Due to the piezoelectric property and high surface energy of ZnO, the pure ZnO is susceptible to be corroded in an acidic environment. Which results in the instability and loss of lifetime for ZnO-based nanodevices. The anti-corrosion methods of materials conclude three main approaches which are the protective cover on the surface, chemical doping and electrochemical protection, respectively. In this work, we adopted the method of indium doping to enhance the anti-corrosion property of ZnO nanobelts in acidic environment. The thickness of the as-synthesized nanobelts is about 30 nm. In the acidic environment ( $\text{PH} \approx 6$ ), the surface morphology, height and electrical transport properties of In-doped ZnO (In-ZnO) nanobelt were relatively stable even after several hours, which showed In-ZnO nanobelt had an excellent anti-corrosion property in acidic environment. Through indium doping, the self-corrosion potential was increased from 0.14 V to 0.172 V. At the same time, the self-corrosion current density was decreased from 17.8 nA/cm<sup>2</sup> to 3.16 nA/cm<sup>2</sup>. It can be apparently seen that the self-corrosion potential of In-doped ZnO nanobelts shifted to more positive values in comparison with pure ZnO nanobelts. In light of such results, this finding is probably to offer a promising approach for fabrication of ZnO-based nanodevices in acidic environment with commercial values.



**Keywords:** ZnO, anti-corrosion, indium doped, nanobelts.

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# Activating the Dull Bimetallic Phosphide via Copper Nanowire Insertion towards Efficient Hydrogen Evolution Reaction

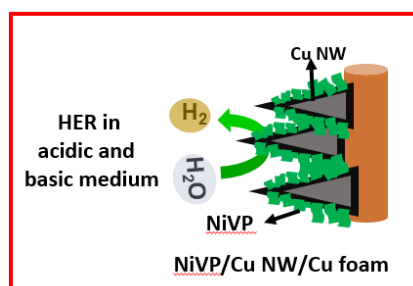
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Electrochemical water splitting is considered to be a new dawn for hydrogen economy, therefore the quest for designing cheap, efficient and stable electrocatalysts is a need of this generation<sup>1,2</sup>. Due to the high cost and scarcity of the noble metal catalyst such as Pt and Ir, their large scale commercial applications are restricted as a result, earth-abundant transition-metal oxides, (oxy)hydroxides, phosphides, and carbides have been extensively developed for electrochemical water splitting. Recently, transition-metal phosphides have emerged as a class of promising catalysts for hydrogen evolution reaction (HER), as the P species could trap protons by acting as a base and facilitate the HER. Nevertheless, the designing of highly efficient phosphide catalysts is seldom achieved and still remains a major challenge. Herein, we present a simple and effective strategy to activate the bimetallic NiV phosphide by injecting the electron from metallic Cu nanowire support underneath the phosphide towards HER. The activity of the Cu nanowire supported NiVP is significantly boosted than compared to the bare NiVP in both acidic and basic electrolyte solution, suggesting the positive effect of the Cu electron density on the NiVP for water reduction. Our strategy can be employed for enhancing the performance of the electrocatalyst and achieving state-of-the-art activity in different energy conversion and storage applications.



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# Oxidation-resistive two-dimensional dihafnium sulfide electride with efficient electrocatalytic activities in water-based solution

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Electrides are exotic ionic crystals where excess electrons are located in cavities as anions. Because of the loosely bound anionic electrons, electrides have been received much attention, exhibiting intriguing physical and chemical phenomena, such as low work function, high electron mobility and excellent catalytic reactivity<sup>1,2</sup>. However, the electro-active functionalities of electrides have been degraded once oxygen and/or moisture is absorbed, preventing the novel applications for an industry. It is thus highly demanded to discover a thermally or chemically stable electride in ambient or moisture condition. Here, we report the highly oxidation-resistive dihafnium sulfide ( $[\text{Hf}_2\text{S}]^{2+ \cdot 2e^-}$ ) electride with efficient hydrogen evolution electrolysis (HEE) activities over 5,000 cycles in water. We have grown single-crystalline  $[\text{Hf}_2\text{S}]^{2+ \cdot 2e^-}$  electride with floating zone (FZ) melting method. X-ray photoelectron spectroscopy (XPS) and electron energy loss spectroscopy (EELS) combined with density functional theory (DFT) calculations clarify that  $[\text{Hf}_2\text{S}]^{2+ \cdot 2e^-}$  electride has two excess electrons per formula unit, which are confined in the Hf-Hf interlayer with dumbbell-like shape.  $[\text{Hf}_2\text{S}]^{2+ \cdot 2e^-}$  electride shows a state-of-the-art durability against air and water among the existing electrides, retaining the crystal structure and physical/chemical properties over 1 month. Furthermore, Cu-loaded  $[\text{Hf}_2\text{S}]^{2+ \cdot 2e^-}$  electride shows highly effective HEE performances comparable to the defect-rich MoS<sub>2</sub>, which is one of the most effective catalyst except Pt for water splitting<sup>3</sup>. Transmission electron microscopy (TEM) observation indicates that the formation of thin native amorphous HfO<sub>2</sub> layer, known as oxidation-resistive passivation layer, is responsible for the electro-catalytic activity in water. It is verified that the anionic electrons of  $[\text{Hf}_2\text{S}]^{2+ \cdot 2e^-}$  electride can migrate to the Cu nanoparticle through the amorphous HfO<sub>2</sub>. Our findings provide an important insight into the design strategy of new oxidation-resistive electrides and their active functionality in electro-chemistry.

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# Dual Function of Metal doped B-TiO<sub>2</sub> without Hole Scavenger for Complete Degradation of Nerve agent

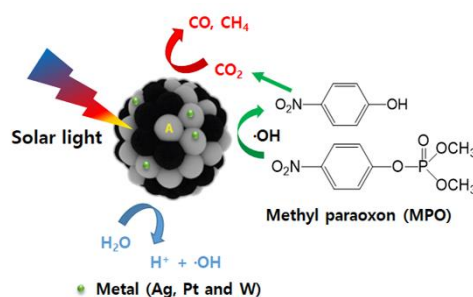
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Up to now, a complete water splitting reaction under sunlight for the photo catalytic processes has been one of the most attractive methods to solve the future energy problems in the world. The complete water splitting is occurred both valence band (VB) for oxidation and conduction band (CB) for reduction on semiconductor materials. However, the complete water splitting reaction requires sacrificial agents for hole scavenger such as methanol at the VB site and for electron scavenger such as AgNO<sub>3</sub> at the CB site [1]. For the complete degradation of organic molecules using photocatalytic semiconducting materials such as TiO<sub>2</sub> [2], both activities at the VB and CB sites are quite necessary for the continuous and complete degradation to oxidation/reduction processes without using any sacrificial scavengers.

In this report, we provide new photo-catalytic dual processes through in-situ degradation of nerve agents to CO<sub>2</sub> at VB site and simultaneously CO<sub>2</sub> conversion to CO and CH<sub>4</sub> at the CB site. Our new blue TiO<sub>2</sub> (B-TiO<sub>2</sub>) has an disordered rutile/ordered anatase TiO<sub>2</sub> phase-mixed structure via lithium-ethylenediamine (Li-EDA) treatment. The methyl paraoxon (MPO) has been known as mimic nerve agents, which is one of sarin simulants that have organophosphorus materials and toxic to human body. Degradation of MPO is occurred on VB site of B-TiO<sub>2</sub> to CO<sub>2</sub> and the resulting CO<sub>2</sub> was gradually converted to CO and CH<sub>4</sub> on CB site of B-TiO<sub>2</sub>. We can achieve 100 % degradation of the MPO nerve agents at CB site and 72.09 % of conversion from CO<sub>2</sub> to CO and CH<sub>4</sub> (615.24 and 307.62  $\mu$ mol/g) at VB site of TiO<sub>2</sub>. It is first time to report for CO<sub>2</sub> reduction from nerve agents by using TiO<sub>2</sub>-based materials. As a whole, our concept can be applied for various environmental, military and energy conversion fields.



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# Visible light mediated C-C bond formation by a single Blue TiO<sub>2</sub> based photo-chiral catalyst

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Photocatalysis has emerged as one of the best strategies for the development of sustainable and novel processes for the synthesis of organic compounds.<sup>1</sup> Although there is enormous growth in this area, the vast majority of the developed methodologies provides achiral or racemic mixture of compounds using either metallic complexes or organic molecules as the photocatalysts. The main reason for this is the difficulty of combining a chiral catalyst to achieve a stereo chemical control, with high reactivity and low activation barriers of radical intermediates.<sup>2</sup> In spite of this difficulty, asymmetric photocatalytic transformations have been accomplished by the use of a dual-catalyst approach using a combination of a photo catalyst and a chiral organocatalyst.<sup>3</sup> The use of only one catalyst that combines chirality and photoredox properties is more convenient but more challenging. A series of highly selective transformations in organic synthesis have been published by TiO<sub>2</sub> photocatalysis. Especially, C-C bond formation mediated by TiO<sub>2</sub>-based photocatalysts sometimes displays a similar powerful ability same as mediated by the noble metals including Pd, Ru, Ir, and Rh based catalysts. But, because of large band gap (3.03-3.20eV) TiO<sub>2</sub>, the organic reactions have occurred only in the presence of UV light.

Here in this work, we have modified the TiO<sub>2</sub> to obtain Blue TiO<sub>2</sub> and then we functionalized the surface with a chiral ligand to form a single photo-chiral organic catalyst. We expect that this single catalyst known as heterogeneous photocatalyst can be applied for the visible light mediated C-C bond formation. We carefully propose the organic reactions to the direct asymmetric photocatalytic visible light C-H functionalization of toluene and its derivatives with high enantiomeric excess, which is a great challenging.

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# Role of Phase-Selective Defects in TiO<sub>2</sub> on Organic Photoreaction under Visible Light

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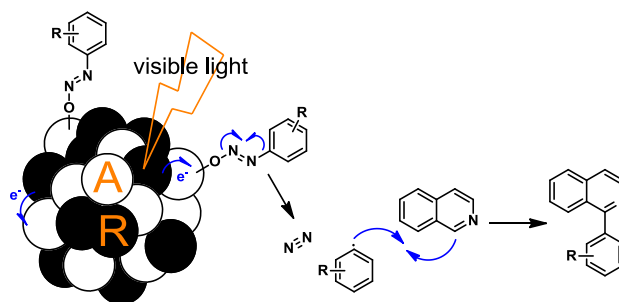
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Titanium dioxide (TiO<sub>2</sub>) is well-known photocatalyst but its applications for organic photoreactions have been limited due to the low absorption of visible light which is more proper energy source for organic synthesis than ultraviolet.[1] Here, we phase-selectively introduce the oxygen vacancies on TiO<sub>2</sub> to enhance the visible light absorption and modulate the molecular adsorptivity.[2]

In the arylation of isoquinoline with aryl diazonium salts under CFL lamp (10 W) as visible light source,[3] Li-EDA treated P25 (ordered anatase/disordered rutile) showed the highest reactivity. Even though oxygen vacancies enhanced the visible light absorption due to the defect states, the changes in surface structure induced the different surface chemistry including the molecular adsorptivity.[4] The oxygen vacancies on rutile phase to enhance the visible light absorption, while crystalline structure of anatase phase was maintained for molecular adsorption, is best condition for the arylation under visible light.



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## Inherently negatively charged copper nanoparticles with oxidation resistance

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Instability of copper toward oxidation hinders widespread use of copper nanoparticles (Cu NPs) in industry [1]. Even though intensive efforts have been made to passivate Cu surface with capping agents, these approaches could not achieve ultimate prevention of oxidation [2,3]. Here, Cu NPs are synthesized onto electrides, which act as a support and a reducing agent for Cu NPs by providing its anionic electrons. Cu NPs grown onto electride are thoroughly investigated using transmission electron microscopy (TEM) accompanied with electron energy-loss spectroscopy (EELS) and X-ray photoelectron spectroscopy (XPS) revealing that Cu NPs preserve its metallic surface over a month. This oxidation resistive behavior is originated from the intimate contact between Cu and electrides, which supplies abundant electrons to Cu NPs, inducing them to be negatively charged. The obtained results suggest that rational protection of Cu against the oxidation in ambient air can be effectively attained by modulating the intrinsic structure and electron density of metal via the use of electrides.

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# Green phosphorus with high mobility and tunable direct band gap

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Black phosphorus can be exfoliated to a few layers, belonging to the class of 2D materials. Exfoliated black phosphorus has received much attention because of its high carrier mobility and moderate band gap which are promising for applications to nanoelectronic and nanophotonic devices. Besides black phosphorus, phosphorus has a polymorphism such as red, white, and violet phosphorus. Recently, blue phosphorene, one of the theoretically suggested P allotropes, has been successfully synthesized on gold substrate. The existence of a variety of phosphorus allotropes motivates our work to search for a new allotrope that provides more interesting characteristics than black phosphorus.

Here we report the discovery of a new P allotrope, called green phosphorus, using a combined approach of global optimization with density functional theory calculations [1]. Green phosphorus has a layered structure with the interlayer interaction comparable to that of black phosphorus. Thus, it should be exfoliated to a few layers, termed green phosphorene. When the film thickness decreases from bulk to monolayer, the band gap increases from 0.7 to 2.4 eV, without altering the direct band gap nature. Green phosphorene exhibits high n-type mobility as well as strong anisotropy along zigzag and armchair directions, suggesting that this allotrope is suitable for novel device applications. Last but not least, we discuss the effects of temperature and substrate on the possible synthesis of green phosphorus.

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## Possibility to find Enantiomeric Excess in Organic Reactions by using Circularly Polarized Light

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To have a high enantiomeric excess (ee) compound in organic synthesis has been extremely important issues since each enantiomer exhibits different physiological activity [1]. To obtain the high ee value through photo-catalytic reaction especially the Diels-Alder reaction has been enormously difficult challenges mainly due to difficult control of the chirality of the radical intermediates. Nowadays, the main way of enhancing the value of ee is forcing on using the chiral compounds in the field of organic photocatalyst. For examples, the photocatalysts like Ruthenium(II) polypyridyl complexes, asymmetric organocatalysts and some chiral transition catalysts show the vital roles to control the ee values. With the irradiation of light, the photocatalysts can facilitate the generation of the radical intermediates in chiral center for increasing the high ee [2].

In this work, we like to introduce on how to approach for controlling the enantiomeric excess of chiral compounds with a help of circularly polarized lights. We expect that the circularly polarized light (CPL) source can give a direction of chirality of the desired product.

# Solution processable ReS<sub>2</sub>-molecular Z-scheme-TiO<sub>2</sub> for excellent solar hydrogen generation by fast charge transfer through multiple junctions

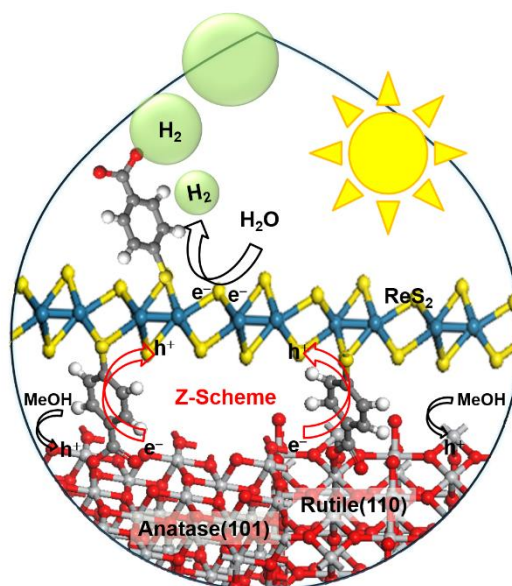
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Effective charge separation and rapid transport of photogenerated charge carriers in semiconductor photocatalysts are required for high efficiency of solar hydrogen generation rates. Here, we report that efficient Z-scheme junctions between two-dimensional rhenium disulfide (2D ReS<sub>2</sub>) and zero-dimensional TiO<sub>2</sub> (0D TiO<sub>2</sub>) result in balanced charge transport of charge carriers generated by the absorption of solar light. For efficient charge transport, multiple junctions of the hydrophilic ReS<sub>2</sub> nanosheets functionalized with benzoic acid onto the two-phased TiO<sub>2</sub> are formed by the condensation reaction between the terminal –COOH groups of ReS<sub>2</sub> and –OH groups of TiO<sub>2</sub>. This new Z-scheme pathway in ReS<sub>2</sub>–C<sub>6</sub>H<sub>5</sub>C(=O)–O–TiO<sub>2</sub> (ReS<sub>2</sub>–BzO–TiO<sub>2</sub>) leads to high photocatalytic activity (9.5 mmol h<sup>–1</sup> per a gram of ReS<sub>2</sub> nanosheets) toward solar hydrogen generation with high cycling stability. Our results provide an effective junction to transfer photogenerated charge carriers rapidly between photocatalytic semiconductors.



# The effect of Li and Ag intercalation to MoS<sub>2</sub> for memory device

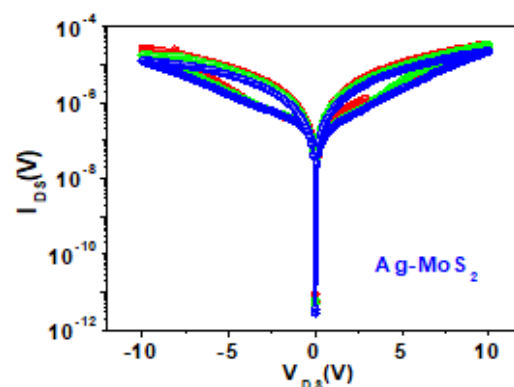
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Graphene and transition metal dichalcogenide(TMDC) are 2D dimensional materials that are actively studied recently for developing various next generation devices. Among the various next-generation device research fields, a two-terminal memory device for implementing a low-power neuromorphic system imitating a human brain has received attention. Unlike the conventional memory device using a three-terminal transistor composed of a drain, a source, and a gate electrode, a two-terminal memory device has a merit in simplifying a device and consuming power because a memory characteristics is shown by voltage control of a drain and a source electrode. The present study aimed at realizing a two-terminal memory device which causes channel or contact resistance change through the movement of intercalated ions through metal ion intercalation of MoS<sub>2</sub>, one of the transition metal chalcogen compounds.

We performed experiments using Li, which is the most commonly used metal in the study of metal ion intercalation between layers in MoS<sub>2</sub>. However, as a result of I<sub>DS</sub>-V<sub>DS</sub> measurement of a MoS<sub>2</sub> intercalated with Li ions, only a phase change (semiconductor → metallic) is observed, and hysteresis for implementing a memory device cannot be seen. In order to solve this problem, we perform additional Ag ions intercalation. After the Ag intercalation, we confirm the formation of hysteresis. The formation of this hysteresis is expected to be due to changes in contact resistance or channel resistance due to the flow of Ag ions. The result of the formation of the hysteresis following intercalation is expected to be useful as a next-generation two-terminal memory, which is worth further research..



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# Dual Vacancies Engineering of 2D MnO<sub>2</sub> for Overall Water Splitting

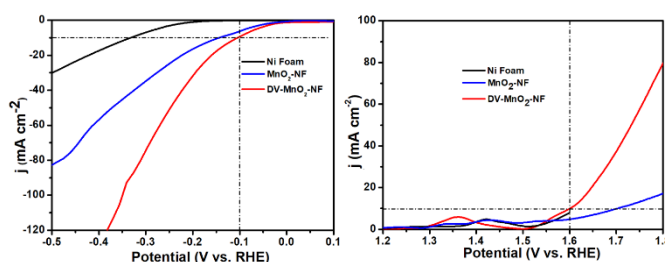
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Until now, Pt for a hydrogen evolution reaction (HER) and IrO<sub>2</sub> for an oxygen evolution reaction (OER) are the most efficient electrocatalysts, but their widespread use for an industrial scale water splitting is still limited due to their high cost and scarcity. Therefore, it is highly desirable to develop efficient low-cost non-noble metal electrocatalysts based on earth-abundant elements for an overall water splitting<sup>[1]</sup>. A layered manganese dioxide ( $\delta$ -MnO<sub>2</sub>) demonstrates very attractive OER performance, especially for mass application. However, it shows unpromising HER performance due to its unsuitable electronic structure and low conduction band level. The layered MnO<sub>2</sub> nanosheets doped with cation and anion dual vacancies ( $V_{Mn}$  and  $V_o$ , denoted as DV-MnO<sub>2</sub>) can have half-metallic properties from semiconductor character and also favourable H<sub>2</sub>O adsorption<sup>[1]</sup>, inspiring a possible



way for the overall water splitting.

Herein, we report the as-prepared ultrathin MnO<sub>2</sub> nanosheets with DV properties in a mild condition. It was carefully designed to prepare the layered DV-MnO<sub>2</sub> nanosheets by introducing new concept, double vacancies of ligand and metal sites of 2D transition metal-based materials. The half-metallicity of MnO<sub>2</sub> attributed to the optimized conduction band edge and wide ranges of  $V_{Mn}$  and  $V_o$  concentrations was expected to provide an excellent electrical conductivity and also rich H<sub>2</sub>O electrocatalytic reaction sites for overall water splitting. The layered DV-MnO<sub>2</sub> nanosheets prepared by a strong reducing agent (lithium-ethylenediamine) system exhibited excellent electrocatalytic performance for both HER and OER with low overpotentials of 100 and 380 mV (in 1M KOH) at 10 mA cm<sup>-2</sup>, respectively, as shown in Figure. Our new concept using the double vacancies in nanosheets can be applied for various kinds of applications including the complete water splitting.

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## Chemical strain formation through anion substitution in ternary transition metal chalcogenides for efficient hydrogen evolution reaction

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To date, researchers have revealed that the electrocatalytic activity can be improved by creation of defects in the crystal lattice of 2-dimensional layered, transition metal chalcogenides (TMCs) such as MoS<sub>2</sub> or Cu<sub>2</sub>MoS<sub>4</sub>, respectively. However, the role of anion substitution for the enhancement of overall electrocatalytic activity in the ternary TMCs (TTMC) remains unproven. Here, we show the substitution of anion atom sulfur (S) with selenium (Se) in a new electrocatalyst Cu<sub>2</sub>WS<sub>4</sub> for efficient hydrogen evolution reaction (HER) activity. The higher electrocatalytic activity of Cu<sub>2</sub>WS<sub>4</sub> after anion atom substitution can be attributed to the creation of chemical strain in the lattice, which causes an increase of active sites for hydrogen adsorption and desorption. Experimentally, the anion substituted Cu<sub>2</sub>W(S<sub>y</sub>Se<sub>1-y</sub>)<sub>4</sub> sample shows superior electrocatalytic activities with low onset potential of 0.320 V at 10 mA/cm<sup>2</sup> for HER, which is two fold lower than the pristine Cu<sub>2</sub>WS<sub>4</sub> (0.650 V at 10 mA/cm<sup>2</sup>) sample. In addition, after 1,000 cycles with continuous electrolysis in an acid electrolyte for 12 h, the anion substituted samples Cu<sub>2</sub>W(S<sub>y</sub>Se<sub>1-y</sub>)<sub>4</sub> preserves its structure and robust catalytic activity perfectly. As a result, our work demonstrates a new approach for developments of real applications of TMCs in energy conversion.

# Hole Scavenger-free Photocatalytic H<sub>2</sub> Evolution on Highly Uniform

## ‘Pt’ Sub-nanoclusters Embedded on Partially Disordered Blue TiO<sub>2</sub>

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Photocatalytic hydrogen generating materials with efficient light harvesting ability and high solar conversion efficiency has gained tremendous attraction nowadays. However, the commercially available photocatalytic semiconductors required a continuous supply of hole scavenger for hydrogen evolution reaction (HER). Herein, we synthesized uniformly dispersed “Pt” sub-nanocluster embedded on partially defected blue TiO<sub>2</sub> by using tannic acid as immobilizer and employed a simple vapor-solid strategy for hydrogen evolution without sacrificial agent. The defected blue P25 nanoparticles would allow to generate a large amount of photoexcited electrons/holes efficiently in the LED light. Furthermore, the as-prepared tannic acid (TA) reduced Pt nanoclusters anchored on blue TiO<sub>2</sub> dramatically enhance HER performance compared to Pt-doped P25. The blue TiO<sub>2</sub> doped by Pt have 2.17 times higher rate of H<sub>2</sub> generation than Pt-doped P25 as well as high stability after 4 rounds for 8-hour running. A homogeneous loading of Pt sub-nanocluster is confirmed by HR-TEM. The surface area enhancement occurs after loading of Pt on defected TiO<sub>2</sub> that is in agreement of perfect Pt loading in Blue TiO<sub>2</sub>. EPR spectroscopy confirmed that coordinated sites and oxygen-vacant sites in the blue TiO<sub>2</sub> nanoparticles interact with platinum and modify the optical and photocatalytic properties. Our technique of applying the vapor-solid system for HER has the advantage of using a very small amount of water, without metal-leaching as compared to other reported methods. The aforementioned strategy of utilizing the vapor-solid system on atomically doped metal nanoclusters on semiconductor oxide support provides a safe and facile material with suitable device design for selectively photocatalytic Hydrogen fuel generation.

# Birch Reduction of Aromatic Compounds by Inorganic Electride $[\text{Ca}_2\text{N}]^+\bullet\text{e}^-$

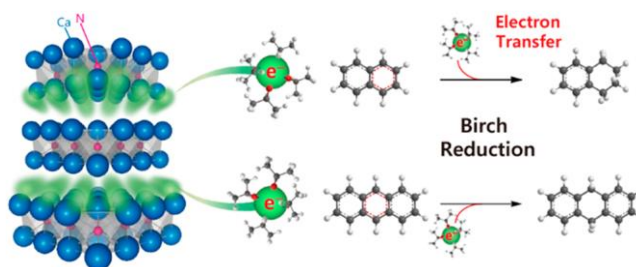
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Birch reduction of aromatic systems by solvated electrons in alkali metal-ammonia solutions is widely recognized as a key reaction because of highly stable conjugated systems. In spite of recent advances in Birch reduction with regard to reducing agent and reaction conditions, there remains an ongoing challenge to develop a simple and efficient Birch reaction under mild conditions. The inorganic electride  $[\text{Ca}_2\text{N}]^+\bullet\text{e}^-$  promotes the Birch reduction of polycyclic aromatic hydrocarbons (PAHs) and naphthalene under alcoholic solvent in the vicinity of room temperature as a solid-type analogy to solvated electrons in alkali metal ammonia solutions.

We propose that an inorganic electride, a solidified crystal of solvated electrons, can provide a powerful new reducing agent for a simple and mild Birch reduction.[1] It is expected to provide a high electron transfer efficiency and environmentally benign processes in universal solvents such as alcohols. The first investigations into Birch reduction using  $[\text{Ca}_2\text{N}]^+\bullet\text{e}^-$  were conducted with anthracene. We utilized the hexamethylphosphoramide (HMPA) solvent as an electron transfer medium, which is known for dissolving alkali metals, generating solvated electrons.[2,3] First, the reducing reaction of the anthracene was examined in HMPA or cosolvent (HMPA/iPrOH) at different reaction temperatures. For the expansion of the reaction scope, we applied the cosolvent systems of THF/iPrOH and HMPA/iPrOH. With the established optimal condition [2 equiv of  $[\text{Ca}_2\text{N}]^+\bullet\text{e}^-$ , THF/iPrOH = 1:1 or HMPA/iPrOH = 1:1, v/v), 65 °C], we examined the Birch reduction of various PAHs and two naphthalene derivatives. This protocol can provide a direct and pragmatic synthetic root for the reduction of aromatic compounds. It also can provide a powerful alternative reducing agent for synthetic chemistry as an analogue of solvated electrons in alkali metal ammonia or amine solutions.



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# Large area sputtered ReS<sub>2</sub> film for optoelectronics

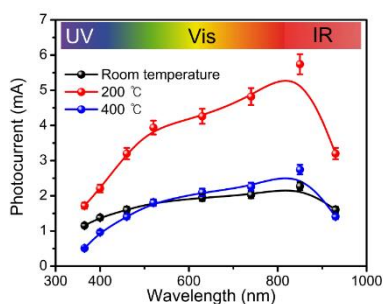
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Transition metal dichalcogenides (TMDCs) have been studied intensively due to their remarkable electrical and optical properties [1]. However, the most of TMDC studies in optoelectronic fields were conducted with monolayer due to layer dependence electronic band structure changes. Atomically thin TMDC monolayer (~0.7 nm) limits device performance due to poor total absorbance [2]. Among TMDCs, ReS<sub>2</sub> is best candidate to solve the performance limitation of optoelectronics with TMDCs due to insensitive direct bandgap property [3]. By combining with this property and sputtering techniques for uniform large area film preparation, it will accelerate the commercialization of TMDCs. Herein, we prepared ReS<sub>2</sub> sputtering target via solid state reaction and spark plasma sintering process. Synthesized polycrystalline ReS<sub>2</sub> for sputtering target and sputtered ReS<sub>2</sub> film were characterized with XRD, PL and etc. Finally, photodetector consisted of sputtered ReS<sub>2</sub> on p-Si with ITO and Al electrode was fabricated and characterized.



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# Studies of electrochemically deposited Platinum on MoTe<sub>2</sub> for catalytic behavior

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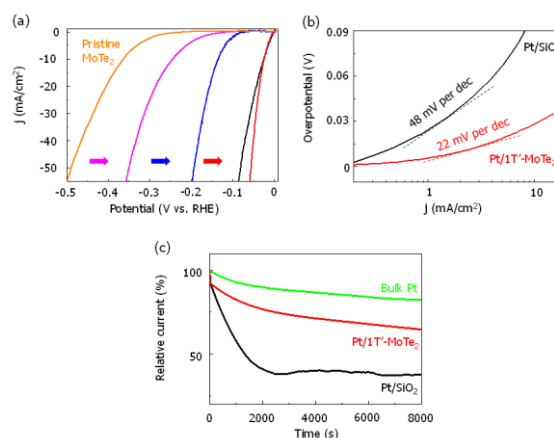
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Electrochemical catalysts based on transition metal dichalcogenides (TMDs) have been intensively studied in hydrosulfurization, hydrogenation, and the hydrogen evolution reaction (HER) [1-3]. Moreover, TMDs have polymorphism, which has stimulated extensive studies on tuning of surface electronic structures for active HER. The polymorphism in TMDs provides an opportunity for new hybrid catalysts with TMDs and other catalytic metals via surface engineering that can create novel facets of the catalytic metals for active HER. Here, we report a hybrid catalyst with monoclinic MoTe<sub>2</sub> and platinum (Pt) for the HER. Pt atoms were decorated on the surface of monoclinic MoTe<sub>2</sub> that has an atomically-distorted lattice structure, which produces a distinct Pt-Te alloy layer. The Pt/MoTe<sub>2</sub> hybrid catalyst exhibits an active HER with a Tafel slope of 22 mV per decade and an exchange current density of 1.0 mA/cm<sup>2</sup>, which are the best values among those reported for TMD-based catalysts. The decoration of catalytic metals on atomically-distorted metallic TMDs realizes rich catalytic active sites on large basal planes for efficient hydrogen production.



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# Nanoporous Graphene membrane for separation

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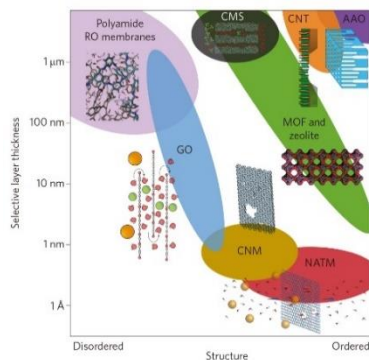
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Membrane separation technology, compared with other separation methods such as distillation and crystallization, has shown its distinctive advantages in energy efficiency and convenience. However, traditional separation membranes are inherently with the trade-off between selectivity and permeance as they are normally made of thick and porous polymers.<sup>1</sup>

Perfect graphene, as an atomically thin material, is physically and chemically stable, mechanically strong and impermeable to all molecules. By selectively removing some carbon atoms in the graphene lattice, it is possible to prepare nanoporous graphene, which can act as an ideal membrane for separation. From theoretical calculation and experimental evidence, nanoporous graphene can achieve higher performance in selectivity and permeance than traditional polymer membranes by several orders of magnitude.<sup>2</sup> Meanwhile, compared with other advanced membrane systems, such as CNM, CNT, CMS, AAO, GO and MOF, nanoporous graphene membrane is potentially with higher selectivity and permeance since it is the thinnest and most ordered among them. (Fig 1)

To prepare high-performance nanoporous graphene, both uniform size in diameter and high density of nanopores in graphene are essential. There are two methods, at present, to prepare nanoporous graphene, which are top-down and bottom-up methods. Top-down methods, including ion bombardment and plasma treatment<sup>3</sup>, can be used to generate nanopores in perfect graphene while bottom-up methods, such as chemical vapor deposition (CVD)<sup>4</sup> and organic synthesis<sup>5</sup>, can directly prepare graphene with intrinsic nanopores.

Currently, we are studying to use both direct CVD synthesis and O<sub>2</sub> plasma post-treatment to achieve precise pore engineering in graphene at the nanoscale. We aim at applying nanoporous graphene membrane for separation of ions and small biological molecules in water, which has great potential in various applications, such as hemodialysis, water desalination and purification, etc.



**Figure 1.** Membrane structure–thickness map with some illustrative examples, including polyamide reverse osmosis (RO) membranes, carbon molecular sieves (CMS), carbon nanotubes (CNT), anodized aluminum oxide (AAO), graphene oxide (GO), metal organic framework (MOF) and zeolite carbon nanomembrane (CNM) and nanoporous atomically-thin membrane (NATM).

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# The Synergistic Effect of Nitrogen Fixation Over Partially Reduced Titanium Dioxide for Solar-driven Nitrogen Conversion to Ammonia

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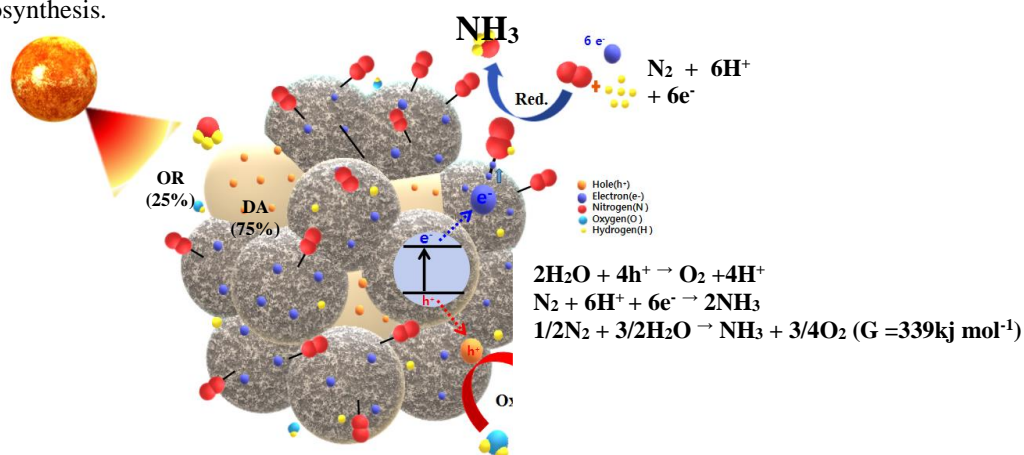
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Ammonia (NH<sub>3</sub>), which is one of the most indispensable carbon-free energy fuels, from water and air by photocatalytic process under mild condition is ideal route to solve fossil fuel combustion and can be alternative way of traditional Haber-Bosch process which requires extensive energy with metal-based catalyst under severe conditions. Several studies have proposed the nitration reduction reaction (NRR\_ mechanism using TiO<sub>2</sub> with a large number of surface oxygen vacancies under UV light, but it has still low efficiency.

Herein, we report excellent photo-catalytic nitrogen conversion to ammonia through nitrogen fixation of nitrogen gas on oxygen vacancies of phase-selectively reduced P25 TiO<sub>2</sub> (disordered anatase (DA)/ordered rutile (OR) phases) nanoparticles. The phase-selectively reduced P25 TiO<sub>2</sub> can provide an excellent light-harvesting performance and efficient separation of charge carriers due to well-formed band alignment of disordered anatase (DA) and ordered rutile (OR) of TiO<sub>2</sub>, promoting largely enhanced catalytic performance (a reaction rate of 2032.5 μmol g<sub>cat</sub><sup>-1</sup> s<sup>-1</sup> and solar to chemical conversion (SCC) efficiency of 0.07 %) under sunlight. Interestingly, apart from DR, nitrogen is merely adsorbed on the oxygen vacant sites on DA. This superior N<sub>2</sub> absorbability of Ti<sup>3+</sup> species on DA facilitates the rate of N<sub>2</sub> reduction and promotes the cleavage of electron-neutral N<sub>2</sub> which is the rate determining step of NRR. Furthermore, controlling a ratio of disordered and ordered surfaces can modulate band gap alignment and charge transport rate into two mixed phases of TiO<sub>2</sub> for better photocatalytic NRR performance. Combination analysis including EPR, BET, Raman spectra verifies linear adsorption of nitrogen with increase of oxygen vacant sites on DA rather than that on DR. Moreover, in-situ diffuse reflectance infrared fourier transform spectroscopy (DRIFT) spectra further demonstrate new mechanism with strong interaction of nitrogen and transition metal that result in fast charge transport to overcome high reductive potential energy of nitrogen triple bond corresponding to excellent catalytic performance toward NRR. This result a considerable potential candidate of engineering for the creation of highly active catalysts owing to its large free-energy gain on defect sites as an artificial photosynthesis.



**Schematic photocatalytic reaction mechanism for NRR on 25% of ordered Rutile and 75% of disordered Anatase of NaP25 under solar light**

# Heterophase Homojunction in single crystal MoTe<sub>2</sub> for Enhanced catalytic Performance

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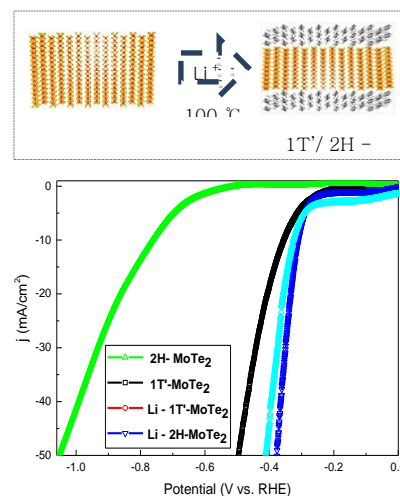
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Beyond Sulfide and selenide-based Transition, metal chalcogenides to have gained recognition as a candidate for emerging application of chemical intercalation and exfoliation [1,2], effort in Tellurium based TMDs looks limited. So far, the introduction of Li<sup>+</sup> changes the local symmetry of the MoS<sub>2</sub>/WSe<sub>2</sub> in favor of the metallic phase, further Li<sup>+</sup> insertion causes the samples to exfoliate down to few-layer regimes, interestingly Monolayer [3]. Unlike MoS<sub>2</sub>, the strong dipole-dipole interaction results in strong interlayer coupling among MoTe<sub>2</sub> layers resulting in large intercalation activation energy across MoTe<sub>2</sub> layers which significantly prohibited chemical intercalation and phase tuning.

We proposed and perform thermal assisted chemical intercalation that could modulate the thermodynamic state of the intercalant ion to overcome activation energy for efficient intercalation in Bulk MoTe<sub>2</sub> that leads to enough charge transfer to surface/subsurface regimes and transform into the Metallic 1T' phases.

Thermal assisted chemical intercalation of bulk single crystal 2H-MoTe<sub>2</sub> and report first chemical phase transition and outstanding electrochemical performance based on same material vertical heterophase architecture. Intercalation temperature and time optimization lead to efficient out of plane and in plane intercalation that induces Metallic phase of MoTe<sub>2</sub> on the top few Layers, while the inner bulk remains semiconducting phase, so-called homojunction heterophase MoTe<sub>2</sub>. We develop a special technique of exfoliation to study the time and temperature dependent phase transition and further verified by XRD and XPS.

In the electrochemical point of view, the heterophase shows substantial enhancement in the overpotential and Tafel slope attributed from significantly lowered charge transfer and improvement of adhesion energy on the outermost strained metallic phase respectively. In the electronic transport property, we observed two order of resistance suppression from its pristine semiconducting counterpart, which found to be a contribution from the outer most metallic phase of the heterostructure. The transport activation energy of the heterophase was 10 times smaller than the pristine single 2H MoTe<sub>2</sub>.



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## Hydrogen bubble-assisted synthesis of reduced graphene oxide-WTe<sub>2</sub> hybrid catalyst for hydrogen evolution

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Carbon-based materials are promising catalyst candidates for electrochemical reactions such as hydrogen evolution reaction (HER). The surface morphology engineering of graphene and reduced graphene oxide (rGO) has been tried to improve the HER, expecting increased catalytically active areas. Until now, the hydrothermal synthesis has been generally used, which requires harsh conditions such as high temperature and pressure and increases the preparation cost. In this work, we developed an efficient electrochemical synthesis of rGO on WTe<sub>2</sub> in a three electrodes setup in H<sub>2</sub>SO<sub>4</sub> solution. A 2.0 V bias was applied to graphite rod to make the graphite surface oxidized, and then the graphite oxide (GO) was exfoliated and deposited on the negatively charged Td-WTe<sub>2</sub> working electrode. As a result, the GO was reduced to rGO and a rGO-WTe<sub>2</sub> heterostructure was formed.

Pristine semi-metal Td-WTe<sub>2</sub> single crystal showed electrochemical catalytic activity in HER with an onset potential of 0.520 V vs. RHE and a Tafel slope of 155 mV/dec. The heterostructure rGO-WTe<sub>2</sub> catalyst showed a much more higher electrocatalytic activity in HER with an onset potential of 0.260 V vs. RHE and a Tafel slope of 39 mV/dec, indicating the Volmer-Heyrovsky mechanism, in which, the hydrogen electrochemical desorption step is the rate-limiting step. In addition, the high double layer capacitance (C<sub>dl</sub>) of 155.2 mF·cm<sup>-2</sup> illustrates the large effective surface area. Compared to the previous reports with carbon-based materials, the higher catalytic performance of rGO-WTe<sub>2</sub> heterostructure in HER might originate from more catalytic active sites on rGO defects resulting from the breaking of C-C or C=C bonds and the formation of C-W bond in synthesis process. The environmentally friendly electrochemical exfoliation and synthesis suggest a great potential on improving the catalytic performance of rGO-based materials in HER.

# Direct Growth of Doping Controlled Monolayer WSe<sub>2</sub> by Selenium-Phosphorus Substitution

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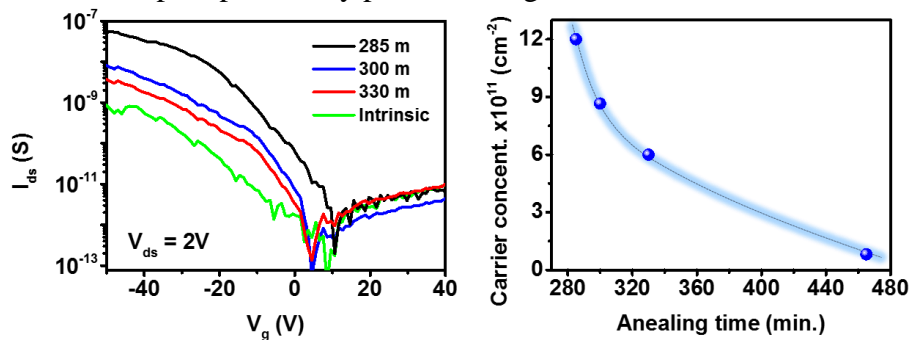
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## Abstract

Transition metal dichalcogenides (TMDs) two-dimensional layered materials (2D) with a superior electrical, optical, and mechanical properties are considered as promising next generation 2D materials in electronic and optoelectronic applications. Tungsten diselenide (WSe<sub>2</sub>) one of those TMDs materials with p-type dominant semiconductor characteristics exhibit a unique indirect to direct band gap transition as decreasing from bulk to monolayer. For the further applications of those TMDs materials, doping is required to control their intrinsic properties like carrier type and range of doping.

Although many studies have been carried out on the doping of transition metal dichalcogenides (TMDs), introducing controllable amount of dopants into TMD lattice is still insufficient. Here, we demonstrate doping controlled TMD growth by replacement of selenium with phosphorus during the synthesis of monolayer WSe<sub>2</sub>. The phosphorus doping density was controlled by fine adjustment of the amount of P<sub>2</sub>O<sub>5</sub> dopant powder along the pre-annealing time. Raman spectroscopy, photoluminescence (PL), X-ray photoelectron spectroscopy (XPS), and high-angle annular bright field Scanning tunneling electron microscopy (HAADF STEM) provide evidence that P doping occurs within the WSe<sub>2</sub> crystal with P occupying the substitutional Se sites. With regard to its electrical characteristics, the hole majority current of P-doped WSe<sub>2</sub> is 100-times higher than that of the intrinsic WSe<sub>2</sub>. The measured doping concentration was ranged from  $\sim 8.16 \times 10^{10}$  to  $\sim 1.20 \times 10^{12}$  depending on the amount of P<sub>2</sub>O<sub>5</sub> dopant powder by pre-annealing.



# Wafer scale continuous bilayer graphene films synthesis by using inductively coupled plasma - chemical vapor deposition

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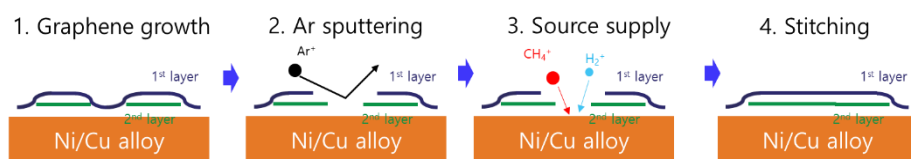
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Graphene has shown a unique combination of unrivaled mechanical and electronic properties which makes it a promising candidate for electronics applications[1]. However, monolayer graphene has a linear gapless band structure. The lack of an energy gap in its electronic structure leads to its low on-off ratio for graphene transistors at room temperature. Bilayer graphene, instead, has an electrical field induced band gap up to 250meV, thus bilayer graphene makes graphene attractive for application such as electronics, terahearth technology, and photonics applications[2].

To date, recent developments in chemical vapor depositions (CVD) methods have allowed successful production of scalable single-layer graphene on metal substrate such as copper. However, the synthesis of uniform bilayer graphene film remains extremely challenging.

Here we report the synthesis of wafer scale continuous bilayer graphene films over 6inch wafer area. The key of our method for achieving a precise control of bilayer graphene layers is the synergetic combination of the remarkably different carbon solubilities of two metals and segregation effects[3]. However, in the above mentioned methods, coverage of bilayers cannot be 100%. For continuous bilayer graphene films, we introduced argon plasma sputtering to etch the 1st layer between 2nd layer domain boundaries. By keeping the carbon and hydrogen supply during 1st layer etching, continuous 2nd layer graphene is successively achieved[4]. This etching and growth approach led to better stitching between 2nd layer graphene domain boundaries. The bilayer nature of graphene film is verified by Raman spectroscopy and atomic force microscopy.



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# Study of defect on atomically thin ReS<sub>2</sub> through chemical treatment effect

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Rhenium disulfide (ReS<sub>2</sub>) is a semiconducting layered transition metal dichalcogenide (TMDs) that exhibit contrasting optical properties compared to the conventional Mo and W based TMDs. A weak inter-layer coupling and stable distorted 1T' phase have been observed in the ReS<sub>2</sub> system.<sup>1</sup> As a result, ReS<sub>2</sub> becomes a direct band gap for all thickness, however the distorted lattice symmetry leads the in-plane anisotropic Raman and PL emission properties.<sup>1,2</sup> Here, we will study the S vacancy states and their healing process on the atomically thin mono (1L), bi (2L) and other thicker layer ReS<sub>2</sub> using the STEM correlated PL and Raman spectroscopy. From our STEM analysis S vacancy states in the 1L as well as multi layers ReS<sub>2</sub> are not easy to detect unlike the case of 1L-MoS<sub>2</sub>.<sup>3</sup> Therefore, no detectable PL enhancement was observed from the 1L ReS<sub>2</sub> as a result of the chemical (TFSI) treatment as shown below, Fig. 1(a). Since, TFSI is well known chemical to increase the PL quantum yield of 1L-MoS<sub>2</sub> to nearly unity by healing the defect states.<sup>4</sup> In contrast, we observed a clear two fold PL enhancement from the bi-, tri- and quad layer ReS<sub>2</sub> due to TFSI treatment effect. This unique result might be associated with the lattice engineering due to weaker inter-layer system of ReS<sub>2</sub> crystals than the defect state healing due to chemical treatment effect. Details will be presented.

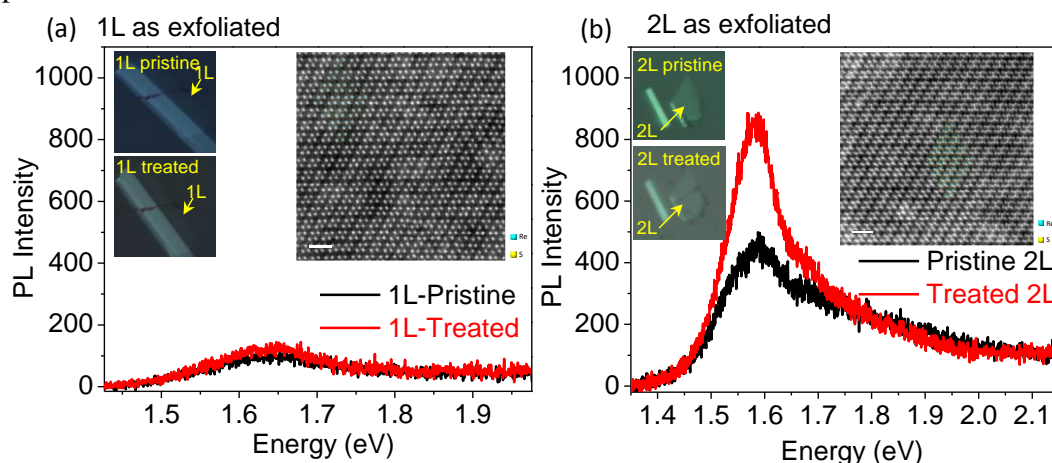


Figure (a) PL intensity comparison of pristine and TFSI treated 1L-ReS<sub>2</sub> using 514 nm laser excitation. Inset of (a) shows optical and STEM Images of 1L-ReS<sub>2</sub> (b) PL intensity comparison of pristine and TFSI treated 2L-ReS<sub>2</sub>. Inset of (b) shows optical and STEM Images of 2L-ReS<sub>2</sub>.

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## Microscopic Origin of Vacancy Healing in Two-Dimensional Semiconductors via Chemical Treatment

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Chemical treatment using bis(trifluoromethane) sulfonimide (TFSI) has been shown to be particularly effective for increasing the photoluminescence (PL) of monolayer (1L) MoS<sub>2</sub>, suggesting a convenient method for overcoming the intrinsically low quantum yield of this material. However, the underlying atomic mechanism of the PL enhancement has remained elusive. We report the microscopic origin of the defect healing observed in TFSI-treated 1L-MoS<sub>2</sub> through a correlative combination of optical characterization and atomic-scale STEM, which showed that most of the sulfur vacancies were directly repaired by the extrinsic sulfur atoms produced from the dissociation of TFSI, concurrently resulting in a significant PL enhancement. DFT calculations confirmed that the reactive sulfur dioxide molecules dissociated from TFSI can be reduced to sulfur and oxygen gas at the vacancy site to form strongly bound S-Mo. Our results underline how defect-mediated nonradiative recombination can be effectively eliminated and provide definitive explanation for the mechanism of the PL enhancement by a simple chemical treatment method, propelling the practical applications of monolayer semiconductors.<sup>1</sup> Details will be presented.

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## Fabrication of perovskite films using solvent engineering with CsPbBr<sub>3</sub> seed crystallization

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Organic-Inorganic hybrid perovskites have attracted tremendous attention as promising materials for light emitting diodes owing to their outstanding optoelectronic performance and low-cost fabrication process. However, polycrystalline perovskite thin film possess disadvantages such as high trap density and small grain size which limit the device performance. Here, we suggest uniform and dense FAPbBr<sub>3</sub> perovskite films fabrication process by solvent engineering treated with CsPbBr<sub>3</sub> quantum dots drop casting to breakthrough these limits. CsPbBr<sub>3</sub> QDs act as stable seed materials during the crystallization process of perovskite films which improves the quality of its device performance. We found that the seed size affects the optical behavior and surface morphology of perovskite films. We confirmed by TEM that the size of CsPbBr<sub>3</sub> QDs can be tuned by adjusting the density of the precursor while QDs manufacturing process. We fabricated FAPbBr<sub>3</sub> perovskite films with various CsPbBr<sub>3</sub> QDs seed condition and conducted PL measurement. We found that the PL intensity of QDs seeded perovskite films is maximum 3 times higher than compared to toluene drop casted perovskite film. We also confirmed by SEM that the grain size of perovskite films is getting bigger with increasing the size of CsPbBr<sub>3</sub> QD seeds. These results provide effective strategy for forming high quality perovskite films for light emitting device.

# Blue TiO<sub>2</sub>/WO<sub>3</sub>/Ag Hybrid nanostructures for Solar light-driven CO<sub>2</sub> reduction into 100% CO

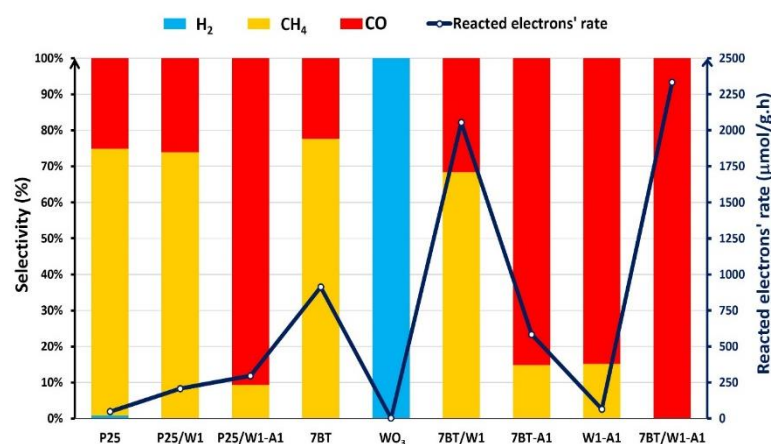
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Photocatalytic reduction of CO<sub>2</sub> into solar fuels is regarded as a promising method to address the global warming and energy crisis problems. Even though the heterostructured TiO<sub>2</sub>/WO<sub>3</sub> catalyst has been known for CO<sub>2</sub> reduction, the selective control for 100% CO product-only remains the subject of debate. Here we report 100% selectivity for CO production-only with enhanced photocatalytic ability using a phase-selectively reduced blue titanium oxide/tungsten oxide–silver hybrid nanoparticles (blue TiO<sub>2</sub>/WO<sub>3</sub>-Ag HNPs) to give 1166.72  $\mu\text{mol g}^{-1} \text{h}^{-1}$  with apparent quantum yield of 34.8%. The construction of a Z-scheme between our blue TiO<sub>2</sub> and WO<sub>3</sub> domains with an excellent band alignment, providing remarkably improved separation of photoinduced charges. Importantly, the presence of novel Ag not only gives the highest selectivity upto 100% CO production-only, but also increases the photocatalytic electron reaction rate (2333.44  $\mu\text{mol g}^{-1} \text{h}^{-1}$ ).



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# Carbon-nanotube based hybrid composite superconducting wire

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The development of superconducting wires is important in terms of energy consumption point. Despite its high potential of application, its utilization is limited by the fabrication processing or mechanical properties of the material. So, to solve this problem, we have fabricated superconducting nanowire yarn to improve the mechanical properties while maintaining the inherent characteristics of superconducting materials.

We show the fabrication of superconducting nanowire yarn by using carbon-nanotube (CNT) based yarn combined with niobium nitride (NbN) which is one of the well-known superconducting materials. CNT based template has been extensively studied due to its various properties such as high flexibility and superior mechanical properties. Here, we used a sputtering deposition for good quality NbN film on CNT sheets and twisted it to make yarn. It shows the superconducting properties, which is similar to those of NbN films. We also confirmed the excellent mechanical properties by test tensile strength and flexibility. Additionally, by adding a low resistivity material to reduce the resistance in the normal state, we designed different structural superconducting cable from the conventional superconducting cable.

These results show the potential application possibility for a new large-scale fabrication technique of flexible, mechanically robust, high-performance superconducting wire.

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# The Effect of Alcohol Solvent on the Synthesis of MoS<sub>2</sub> Quantum Dots with Solvothermal method

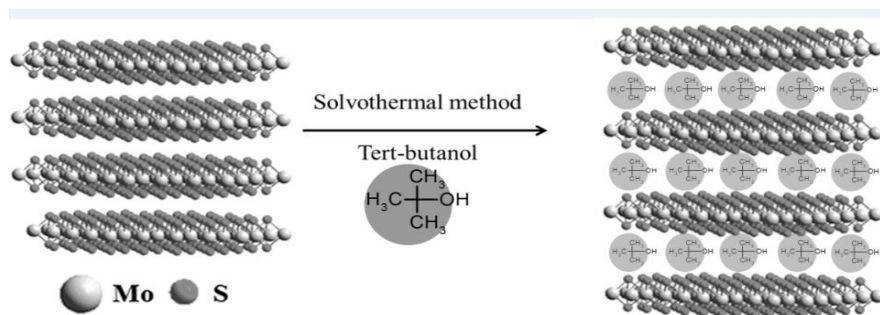
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Graphene, having atomically thin layered structures of two-dimensional (2D) materials, has come into the spotlight over the past few years due to its abundant properties. [1] However, the limitation of the zero band gap has led to research of other 2D materials.[2] In particular, TMDs that consist of a sandwich bonding structure of a single layer transition metal between two layers of chalcogens, have attracted significant attention for decades. Because TMDs are not only layered semiconductors weakly bonded by van der Waals' interaction, but showing a various range of mechanical, electronic, chemical, optical and thermal characteristics. Especially, MoS<sub>2</sub> QDs has appeared and focused on significant research interest as a new type of QDs.



In this study, we report one-pot direct synthesis of molybdenum disulfide (MoS<sub>2</sub>) quantum dots (QDs) from each powder. This solvothermal method using alcohol solvents does not require a purification process of residue such as a metal intercalation, which is a simple and eco-friendly method leading to the successful reduction of waste solvents for the purification. Also, this result gives a clue to develop a product yield with a methyl (CH<sub>3</sub>) group. MoS<sub>2</sub> QDs with the lateral size in range of 1-4.5 nm and exhibited a blue luminescence under 365 nm ultraviolet (UV) light irradiation. Their height level was 0.68-3 nm which correspond to few layers of MoS<sub>2</sub>. This QDs showed a clear atomic lattice structure, and slightly shifted Raman spectra. Such results are due to parameters of each bulk, possibly led by the 0D structure and decrease of layer-layer interactions.

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## Large-area and low-temperature synthesis of few-layered WS<sub>2</sub> films for photodetectors

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Tungsten disulfide (WS<sub>2</sub>), which is one of the 2D materials, has excellent electrical and optical properties. WS<sub>2</sub> thin films show a thickness dependent band gap ranging from 1.3 eV (bulk) to 2.1 eV (monolayer). Furthermore, WS<sub>2</sub> shows one order of magnitude higher absorbance than GaAs and Si in the thickness of ~1 nm. Due to its attractive optical properties, WS<sub>2</sub> has been attempted to grow large-area with high uniformity but the difficulty in synthesizing of WS<sub>2</sub> is an obstacle.

In this work, we fabricated WS<sub>2</sub>-based photodetectors by RF magnetron sputtering and EBI without additional substrate heating, and characterized the structural, compositional, and photoelectrical properties of the synthesized WS<sub>2</sub> films. These analyses revealed successful transformation of the as-deposited sample from an amorphous film to a uniform 2D layered crystalline structure over a 50.8 mm wafer after 1 min of EBI. Furthermore, after the EBI process, PL peaks were observed at 1.89 and 2.06 eV, and the responsivity (R) of the WS<sub>2</sub>-based photodetectors increased. The as-deposited sample showed an R value of 0.10 mA·W<sup>-1</sup> under 450 nm laser illumination, which increased to 0.36 and 1.68 mA·W<sup>-1</sup> for the 1 kV and the 3 kV samples, respectively. The R values of the 1 kV and the 3 kV samples were 1.37 and 2.45 mA·W<sup>-1</sup> at 532 nm, and 0.19 and 1.09 mA·W<sup>-1</sup> at 635 nm, respectively. The increase in the crystallinity and decrease in the resistance after the EBI process increased R. The increase in the absorbance also contributed to an increase in R. EBI is a simple, fast, and controllable method to prepare crystalline

## TMDs-assisted graphene foam/polymer hybrid nano-structures for wearable strain-pressure sensor

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Wearable strain-pressure sensors have gained considerable attention in recent years due to their potential applications in healthcare monitoring and human motion detection. Recent development of 3D graphene with microporous network structure forming graphene porous network (GPN) assisted with supported polymer (Ecoflex) exhibited excellent electrical and mechanical stability. Furthermore, transition metal dichalcogenides (TMDs) such as MoS<sub>2</sub>-based piezo-resistive sensors are well known for their excellent mechanical properties and high gauge factor.

Herein, we demonstrate a flexible and highly sensitive strain-pressure sensor based on TMDs-assisted graphene foam/Ecoflex hybrid nanostructures. The hybrid nanostructures consist of a molybdenum disulfide (MoS<sub>2</sub>) formed as MoS<sub>2</sub> planner sheets on GPN, resulting in enhancement of sensing performance. The MoS<sub>2</sub> planner sheets were uniformly arranged with a cracked-paddy shape on the GPN, and the size of nanoflakes formed on MoS<sub>2</sub> planner sheets was gradually enlarged by increasing the concentration of (NH<sub>4</sub>)<sub>2</sub>MoS<sub>4</sub> solution. In our finding, these conformal nanostructures of MoS<sub>2</sub> on the GPN can produce improved resistance variation against external strain and pressure. The presence of the graphene and MoS<sub>2</sub> were confirmed in MoS<sub>2</sub>/GPN/Ecoflex by a Scanning Electron Microscopy/Energy Dispersive X-Ray Spectroscopy (SEM/EDS), X-ray photoelectron spectroscopy (XPS) and Raman analysis. Consequently, our MoS<sub>2</sub>/GPN/Ecoflex sensor exhibited noticeably improved sensitivity compared to previously reported GPN/PDMS sensors in a pressure test due to the existence of the MoS<sub>2</sub> planner sheets. Notably, the MoS<sub>2</sub>/GPN/Ecoflex sensor showed a high sensitivity of ~6 kPa<sup>-1</sup>. Additionally, it showed excellent durability even under repeated loading-unloading pressure and bending over 4000 cycles. This study paves the way to apply for next-generation wearable electronic devices.

# Microstructural Evolution of Sputtered SnS<sub>2</sub>, SnS Thin Films by Room Temperature Electron Beam Irradiation

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Recently SnS<sub>2</sub> and SnS are as much as powerful candidates of future material for nano-electronic devices compete with other transition metal dichalcogenides (TMDs). Since the band gap of SnS<sub>2</sub> is 2.48 eV, compare with MoS<sub>2</sub> (1.9 eV) or WS<sub>2</sub> (2.1 eV) SnS<sub>2</sub> has the advantage to solve a short channel issue. The large band gap of SnS<sub>2</sub> is proper for consisting multi-purpose of heterolayer which consists of 2 or more types of TMDs. The band gap of SnS thin film is 1.35 eV and the absorption coefficient is about  $10^5$  in the visible region. Furthermore SnS exhibit an intrinsic p-type semiconductor characteristic against most of TMDs. Obtaining highly ordered thin film SnS<sub>2</sub>, SnS could achieve by relatively low temperature because of its melting temperature is about 700°C lower than other TMDs. And earth-abundant and low-cost characteristics of tin sulfide compounds may cater well to the industrial requirements for mass production.

In the present research, short-term E-beam irradiation (EBI) has been conducted at room temperature for crystallization and phase transformation of SnS and SnS<sub>2</sub>. We fabricated an as-deposited SnS<sub>2</sub> thin film by RF sputtering and evaluated the characteristics by different deposition conditions. Due to the EBI process, the amorphous SnS<sub>2</sub> thin film had been transformed to crystallized SnS<sub>2</sub> or SnS. In Raman spectrum, the as-deposited sample and EBI crystallized SnS<sub>2</sub> thin film showed 28.10 cm<sup>-1</sup>, 12.08 cm<sup>-1</sup> of FWHM value, respectively. Transformed SnS film was detected by a result of Raman spectroscopy, X-ray photoelectron spectroscopy, and transmission electron microscopy. For improving film quality and forming a uniform phase of each layer, voltage acceleration, working pressure, and a process time of Electron beam were tested. And we optimized the fabrication parameters for the high quality of tin sulfide compounds thin films.

## Wafer-scale few-layer molybdenum disulfide as a multifunctional optical material

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Atomically thin transition metal dichalcogenides (TMDCs) have received substantial interests due to their unique thickness-dependent optical and electronic properties, and related applications in optoelectronics. However, the large-scale, thickness-tunable growth of such materials are still challenging.

Herein, we report a fast growth of 6-inch scale, thickness tunable MoS<sub>2</sub> flakes on common soda-lime glass, by using NaCl-coated Mo foils as metal-precursors. The MoS<sub>2</sub> thicknesses are tuned from one layer (1L) to >20L by controlling the concentrations of NaCl promoters. To attest the ultrahigh crystal quality, related devices based on monolayer–multilayer MoS<sub>2</sub> heterojunctions have been constructed and displayed relative high rectification ratio ( $\sim 10^3$ ) and extra high photoresponsivity ( $\sim 10^4$  A/W). Thanks to the scalable sizes, the applications in bio-compatible culture plates and ultraviolet (UV) irradiation filtering eyewear are also demonstrated. Our work should hereby propel the scalable production of layer-controlled TMDCs, as well as their optical and optoelectrical applications.



### Reference

Pengfei Yang, Zhepeng Zhang, Yanfeng Zhang\*, submitted

## Direct growth of layered antimonene on transition metal dichalcogenides by chemical vapor deposition

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The family of layered Group-VA materials including black phosphorus, bismuthine and antimonene have been attracting interests due to their high carrier mobility and broad range of bandgaps by controlling layer thickness. Especially,  $\beta$ -phase antimonene (Sb) has stable buckled structures and their electronic band structures change from semimetal in a bulk into semiconductor in a single layer or bilayers. This fascinating layered material can give a chance to significantly reduce contact resistance of the heterostructure interfaces when semimetals and semiconductors are stacked with clean interfaces. However, the direct heterostructure growth by chemical vapor deposition (CVD) still needs to improve. Here, we directly synthesized semi-metallic layered Sb onto semiconducting MoS<sub>2</sub> by CVD. Since vertical stacking by direct growth is promising approach for designing advanced functionality for two dimensional materials, epitaxial grown layered Sb onto MoS<sub>2</sub> can be used for Schottky barrier diode or transparent electrode in the future. Furthermore, reducing Sb layer by hydrogen plasma treatment will be discussed.

# Quantum Dots Embedded Hexagonal Iron Oxide for Fiber-Shaped Battery-like Anode

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Nowadays, fiber-shaped electrochemical energy storage devices have attracted great attention due to the wide range of applications, especially in flexible and wearable electronic devices. CNT yarn has owned high-strength, high thermal-electrical conductivity, and flexibility. Many kinds of literature have reported the decoration of specific guest materials on CNT which enhances a lot capacity of fiber-shaped supercapacitor based on CNT [1-2]. Iron oxide ( $\text{Fe}_2\text{O}_3$ ) is well-known negative electrode material offering large potential window as well as high capacity. Moreover, nowadays, carbon dots or graphene quantum dots (GQDs) have been received much attention when combining with metal oxides, which not only increasing the performance but also enlarging the potential window of supercapacitor devices. Herein, by one-pot hydrothermal synthesis, we have succeeded in the fabrication of iron oxide flakes on individual CNT in fiber-shaped yarn structure. After that merely keeping the as-prepared yarn into N-doped GQDs solution, we have fabricated successfully GQDs@ $\text{Fe}_2\text{O}_3$ /CNT yarn electrode. In three-electrode configuration, the  $\text{Fe}_2\text{O}_3$  coated GQDs grown on CNT yarn electrode achieves a capacity of  $395 \text{ mAh cm}^{-2}$  ( $1185 \text{ mF cm}^{-2}$ ) which is 2-fold higher than the  $\text{Fe}_2\text{O}_3$ /CNT yarn electrode without GQDs at the same scan rate of  $5 \text{ mV s}^{-1}$ . In comparison about stable potential window, the GQDs@ $\text{Fe}_2\text{O}_3$ /CNT yarn electrode shows the onset potential for hydrogen evolution reaction (HER) at  $-1.3 \text{ V}$  (vs. SCE) while the  $\text{Fe}_2\text{O}_3$ /CNT yarn only starts HER at  $-1.2 \text{ V}$  (vs. SCE) at  $5 \text{ mV s}^{-1}$ , which may be caused by the formation junction between GQDs and metal oxides, as mentioned in previous report [3]. We expect that kind of structure can be a good candidate for asymmetric flexible supercapacitor.

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# A free-standing SnS<sub>2</sub> nanoparticles/CNT thin film for sodium ion battery anode electrode

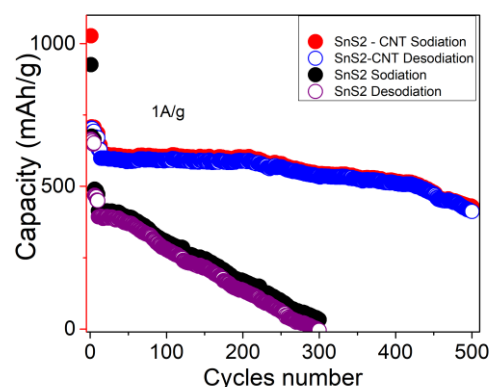
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Sodium ion battery (SIB) has been considered a promising candidate for the grid-scale energy storage applications owing to the abundance and low cost of the precursor[1]. Nevertheless, the inadequacy of high capacity and long life-cycles anode materials hinders the commercialization of SIB. So far, Tin-based compounds have attracted a great concern in SIB development as offering both conversion and alloying process with high theoretical capacity of Na<sub>15</sub>Sn<sub>4</sub> (851 mAh/g)[2]. The volume extension (420%)[3] during the sodiation process and the low conductivity of Sn, unfortunately, still remain as a big challenge in the long cycle-life tin-based SIB development. Hither, we report a simple hydrothermal method to prepare free-standing ultra small (less than 10nm) SnS<sub>2</sub> nanoparticles on CNT thin film to enhance the performance of SIB anode. The hybrid exhibits an excellent cyclability with the capacity of 607 mAh/g after 100 cycles, and 435 mAh/g after 500 cycles at the current density of 1 A/g, demonstrating great capability to be applied for high-performance rechargeable batteries.



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# CsPbBr<sub>3</sub>@metal nanocrystals for photocatalytic application

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Recently, halide-perovskite materials are promising for various applications including optoelectronic devices such as solar cells, photodetectors and phototransistors due to their high absorption density, carrier diffusion length and easy solution process.[1-2] Thus, lots of methods have been developed to change the composition and morphology of the perovskite nanocrystals to modulate the optophysical properties.[3, 4] Especially, dimension of nanocrystals such as nanodots, nanorods, nanowires, nanosheets, and nanoplatelets confines the photogenerated charge carrier and change the charge transport performances.

Here in, metal nanoparticle incorporated CsPbBr<sub>3</sub> nanocrystals with different size confinement is synthesized to control the optical and electronic properties via exciton-plasmon interaction and further to mediate the charge transfer for application of photocatalysts. The optical and electrical properties of these nanocomposites are analyzed using HRTEM, XRD, UV-vis absorption and PL spectroscopy.

## **Keywords**

Perovskite nanocrystals, colloidal synthesis, charge transfer

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# Energetics and bias-dependent scanning tunneling microscope images of intrinsic defects in 2H-MoTe<sub>2</sub>

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MoTe<sub>2</sub> is one of the representative transition metal dichalcogenides (TMDCs) and has been studied extensively due to its high current-on/off ratio implying potential applicability in field-effect transistors [1-5]. In this presentation, we report the energetic stability of various intrinsic defects in three-trilayer (3TL) 2H-MoTe<sub>2</sub>. We performed density functional theory (DFT) calculations by using Vienna ab-initio simulation package in conjunction with the Perdew-Burke-Ernzerhof exchange-correlation functional and the DFT-D3 van der Waals (vdW) correction scheme. A 5x5 surface supercell was used to simulate isolated defects. We examined vacancies, adatoms, interstitials, and intercalations in the vdW gap. The most stable defect is found to be the Te adatom on top of a Te atom of 3TL 2H-MoTe<sub>2</sub>, and its formation energy is 1.06 eV in the Te-rich condition, followed by Te vacancy, Mo vacancy, Te intercalation, Mo interstitial, and Mo intercalation. This is in agreement with a previous study using 1TL MoTe<sub>2</sub> [6]. We simulated the constant-current scanning tunneling microscope (STM) images within the Tersoff-Hamann approximation for the clean 2H-MoTe<sub>2</sub> and intrinsic defects. The simulated STM images show strong bias-dependence, which can be explained by examining the electronic structure (e.g., partial density of states). Such strongly bias-dependent STM images can be used to identify intrinsic defects observed in experimental STM images [7-8].

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## Flexible Broadband Cr/PET/Cr Solar Absorber

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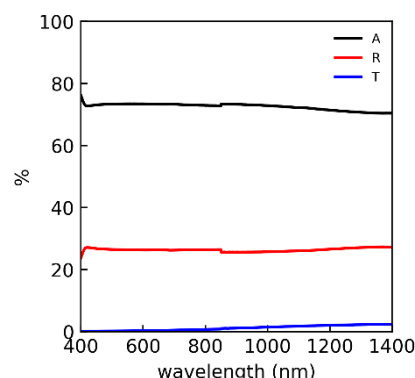
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A metal-dielectric-metal(MDM) structure known as Fabry-Pérot(F-P) resonance is promising for a solar absorber of thermophotovoltaics [1] and thermoelectrics [2] and colored solar cells [3]. Although the MDM absorber also allows the flexibility with flexible substrate [4], general dielectric materials for the transparent middle layer of the MDM absorber easily have cracks even under a weak strain, which inevitably leads to the degradation of their properties as the number of stretching or relaxing cycles increases [2].

Here we demonstrate flexible, broadband and lithography-free optical absorber based on MDM (Cr/PET/Cr) structure. By using UV/VIS absorption spectrometer, we have measured more than 72% absorption over the wavelength range from 400nm to 1400nm. The designed MDM absorber can provide various applications such as the thermoelectric devices, solar cells and structure color filters.



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## Degradation analysis of perovskite films using the photo thermal induced resonance spectroscopy

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Perovskite films based on  $\text{CH}_3\text{NH}_3\text{PbI}_{3-x}\text{Cl}_x$  undergo rapid degradation when exposed to oxygen and moisture. To overcome this issue, many researchers have been studied the degradation mechanism of perovskite films. However, clear degradation mechanism is not solved yet.

In this work, we investigated the degradation mechanism of perovskite films by photo thermal induced resonance (PTIR) technique combined with atomic force microscope (AFM). We reveal that the degradation of perovskite film was easily occurred at grain boundary (GB) than grain interior (GI). Before the degradation, we observed that the intensity of N-H stretch bond of perovskite film was higher at GB than GI. While after the degradation, it was decreased along the GB. After the further degradation, we observed that the intensity of mixed (hydrogen bonded and free O-H) bonds was firstly shown at GB. Overtime, the intensity of mixed O-H bonds was increased both GB and GI. Thus, we confirmed that the degradation mechanism of perovskite film by using the correlated structural, chemical and optical analysis. Finally, this study will contribute to understanding of the mechanism of the degradation process of perovskite films and enhance the stability of perovskite optoelectronics field.

# Multi-functional aligned carbon nanotubes sheet for liquid crystal display device

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The commercial liquid crystal display (LCD) module consist of the polarizer-substrate-transparent conductive film (TCF)-orientation film. Although indium tin oxide (ITO) has been used widely for the TCF, brittle nature of ITO hinders its sustainable application in the flexible display device. Also, the complicated and multi-layered structure raises its unit cost. Therefore, the development of alternative brittle material and simplification if the construction has been studied widely. The carbon nanotubes (CNTs) is an appealing candidate of display component materials owing to their excellent electrical conductivity, anisotropic optical character, extremely high aspect ratio, and superb mechanical properties. Besides, we can artificially modulate their optical and electrical performance through the uniaxial alignment of CNTs. Here, we report the multi-functional aligned CNT sheet for the flexible display application. The highly aligned CNT sheet acted as a linear polarizer under the visible light owing to the anisotropic light absorption of CNT.<sup>1</sup> The degree of polarization (DOP), which defined by  $(T_{\parallel}-T_{\perp})/(T_{\parallel}+T_{\perp}) \times 100$ , of 14 layers CNT/OA composite film is 63.5% at 550 nm wavelength. Also, their sheet resistance shows 530  $\Omega/\square$ , which replaced the function of TCF. The uniaxially and uniformly patterned morphology of film aligned liquid crystal molecules (orientation film). We confirmed a good on/off switching performance of the twisted nematic mode of LCD module fabricated with CNT sheet.

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# **Thermally Reduced Graphite oxide/Carbon Nanotubes Supported Molybdenum Disulfide as Catalysts for Hydrogen Evolution Reaction**

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*Abstract will be updated soon..*

# Wafer-scale single-crystal hexagonal boron nitride film via self-collimated grain formation

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Many studies have been carried out for the synthesis and quality improvement of Hexagonal Boron Nitride(hBN) using chemical vapor deposition[1-4], but the defects of hBN due to the grain boundary of the metal catalyst in the synthesis step are formed. It still causes charge scattering and trap sites, impeding high-performance electronics. In this study, we report a method of synthesizing wafer-scale single-crystalline hBN(SC-hBN) monolayer films by chemical vapor deposition. The limited solubility of boron (B) and nitrogen (N) atoms in liquid Au promotes high diffusion of adatoms on the surface of liquid at high temperature to provoke the circular hBN grains. These further evolve into closely packed unimodal grains by means of self-collimation of B and N edges inherited by electrostatic interaction between grains, eventually forming an SC-hBN film on a wafer scale. This SC-hBN film also allows for the synthesis of wafer-scale graphene/hBN heterostructure and single-crystalline tungsten disulfide.

# Growth and Simultaneous valleys Polarization of Monolayered MoSe<sub>2</sub>-WSe<sub>2</sub> lateral heterostructure

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The non-centrosymmetric monolayer MX<sub>2</sub> (where M: Mo,W and X: S,Se) have two degenerate but inequivalent energy valleys at  $K$  and  $K'$  points in k-space, which make them ideal systems for valleytronics. The valleytronics propose to exploit “valley degree of freedom” of electron beside its spin and charge for information storage and processing by selectively populating them i.e.  $K$  or  $K'$ . In this study, high-quality monolayer MoSe<sub>2</sub>-WSe<sub>2</sub> lateral HSs are grown by pulsed-laser-deposition-assisted selenization method. The sharp interface of the lateral HS is verified by morphological and optical characterizations. Intriguingly, photoluminescence spectra acquired from the interface show rather clear signatures of pristine MoSe<sub>2</sub> and WSe<sub>2</sub> with no intermediate energy peak related to intralayer excitonic matter or formation of Mo<sub>x</sub>W<sub>(1-x)</sub>Se<sub>2</sub> alloys, thereby confirming the sharp interface. Furthermore, the discrete nature of laterally attached TMDC monolayers, each with two valleys marked by ( $K_M$ ,  $K'_M$ ) for MoSe<sub>2</sub> and ( $K_W$ ,  $K'_W$ ) for WSe<sub>2</sub>, allows simultaneous control of the four valleys without any crosstalk effect over the interface. As an example,  $K_M$  ( $K_W$ ) or  $K'_M$  ( $K'_W$ ) valleys are simultaneously polarized by circularly polarized optical pumping, where the maximum degree of polarization is achieved at their respective band edges. Our work provides new growth mechanism of laterally sharp HSs and highlights their potential use in valleytronics.



# ***Abstract***

## **Poster Session Tuesday**

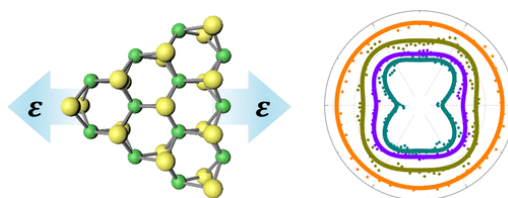
# Monitoring Local Strain Vector in Atomic Layered MoSe<sub>2</sub> by Second-Harmonic Generation

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Strain serves as a powerful freedom to effectively, reversibly, and continuously engineer the physical and chemical properties of two-dimensional (2D) materials, such as bandgap, phase diagram, and reaction activity. Although there is a high demand for full characterization of the strain vector at local points, it is still very challenging to measure the local strain amplitude and its direction. Here, we report a novel approach to monitor the local strain vector in 2D molybdenum diselenide (MoSe<sub>2</sub>) by polarization-dependent second-harmonic generation (SHG). SHG, a second-order nonlinear optical process, is directly related to the lattice symmetry [1]. The strain amplitude can be evaluated from the SHG intensity in a sensitive way (−49% relative change per 1% strain); while the strain direction can be directly indicated by the evolution of SHG pattern [2]. In addition, we employ this technique to investigate the interlayer locking effect in 2H MoSe<sub>2</sub> bilayers when the bottom layer is under stretching but the top layer is free. Our observation, combined with *ab initio* calculations, demonstrates that the noncovalent interlayer interaction in 2H MoSe<sub>2</sub> bilayers is strong enough to transfer the strain of at least 1.4% between the bottom and top layers to prevent interlayer sliding. Our results establish that SHG is an effective approach for in situ, sensitive, and noninvasive measurement of local strain vector in non-centrosymmetric 2D materials.



**Fig.1** Strained monolayer MoSe<sub>2</sub> and corresponding polarization-dependent SHG.

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# Multilayer MoS<sub>2</sub> field-effect transistors using 2-dimensional $\alpha$ -Mo<sub>2</sub>C film as electrodes

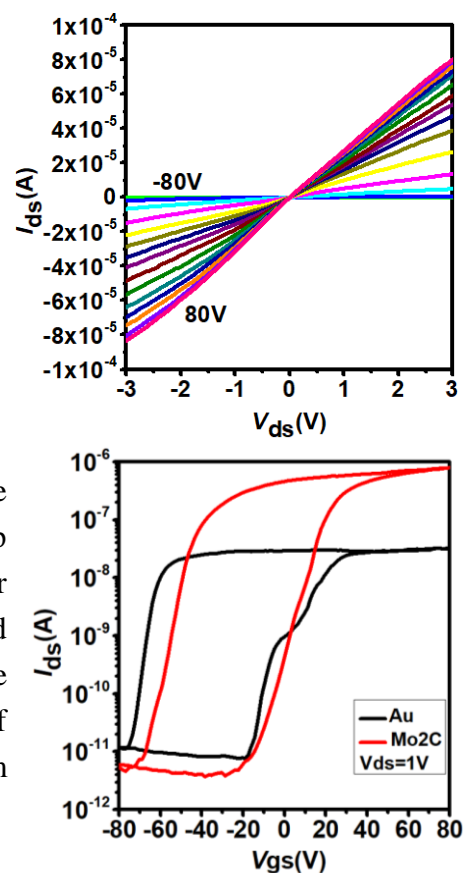
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Low electrical contact resistance is one of major challenges to fabricate high performance field-effect transistors based on two-dimensional transition metal dichalcogenides [1]. Here, we reported high-performance MoS<sub>2</sub> field-effect transistors using 2-dimensional  $\alpha$ -Mo<sub>2</sub>C film as electrodes, exhibiting ohmic contact between multilayer MoS<sub>2</sub> and  $\alpha$ -Mo<sub>2</sub>C at room temperature, as can be seen in the right figure (top). The as-synthesized  $\alpha$ -Mo<sub>2</sub>C crystals were transferred to heavily P-doped silicon substrate with 300 nm SiO<sub>2</sub> [2]. We patterned the  $\alpha$ -Mo<sub>2</sub>C electrodes by using standard lithography process and reactive-ion etching processes. The multilayer MoS<sub>2</sub> were prepared on polydimethylsiloxane (PDMS) stamp by mechanical exfoliation and transferred to the top surface of electrodes. Compared with Au electrodes, the transistor with  $\alpha$ -Mo<sub>2</sub>C electrodes show a much lower contact resistance and a larger on/off ratio of  $10^2$ , as can be seen in the right figure (bottom). The as-fabricated transistors show a carrier mobility of  $50 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  and an on/off ratio greater than  $10^6$  at room temperature.



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2. Chuan Xu<sup>1</sup>, Libin Wang, Zhibo Liu<sup>1</sup>, Long Chen, Jingkun Guo, Ning Kang, Hui-Ming Cheng, Wencai Ren, Nat. Mater. 14, 1135–1141 (2015).

# High-performance phototransistors based on a hybrid channel of CsPbBr<sub>3</sub> quantum dot and carbon nanotube network

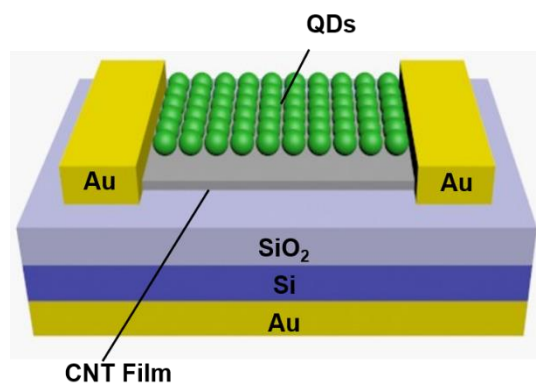
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Perovskite quantum dots (QDs) have been widely used in phototransistor applications [1]. However, the responsivity of the phototransistor is low due to the small charge transport efficiency in QDs layer [2].

Here, we report a phototransistor with a novel structure based on a hybrid channel of CsPbBr<sub>3</sub> QD and carbon nanotube (CNT) network, as can be seen in the figure in the right. Photo-excited carriers are generated by light absorption in the quantum-dot layer, and lead to a remarkable current increasing in phototransistors. The devices exhibit excellent optoelectrical properties in terms of an external quantum efficiency of  $3.0 \times 10^5$ , a responsivity of  $984 \text{ A W}^{-1}$ , a sensitivity of  $> 10^6$ , a detectivity of  $3.52 \times 10^{11}$  Jones and a low dark current of pico-Ampere level. Our presented method can be applied for many other quantum dots photodetectors.



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## Designing nanoscale elastic structures of 2D materials-based electrodes

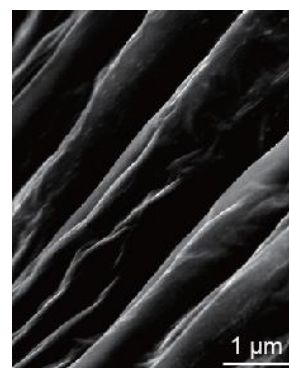
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The emerging flexible and biomedical electronics has motivated the development of the power sources, which have the ability to work normally under large or cyclic deformations [1]. Lithium-ion batteries or supercapacitors are commonly used energy storage devices with quite good performance, making their flexible forms attractive. The various two-dimensional materials, such as graphene or MXenes, can be used to form elastic electrodes due to the intrinsic flexibility [2]. However, the elasticity and long-term stability of 2D materials-based electrodes relies on the deformable structure rather than 2D materials themselves, as the sheets tend to aggregate during formation and lose their flexibility [3].

Here, we design a strain self-engineering method that uses compressive stress induced in the processing of 2D materials to form elastic micro-structures, which will keep the flexibility. For example, thermochemical reactions formed  $\text{MoO}_3$ -g- $\text{C}_3\text{N}_4$  films spontaneously form self-organized nanoscale wrinkles, because of the lamellar structure and reaction-induced internal stress [4]. And compared to the smooth  $\text{MoO}_3$  film, the  $\text{MoO}_3$ -g- $\text{C}_3\text{N}_4$  film shows an obvious brittle-ductile transition and a 1300% stretchability improvement as a result of its wrinkled morphology. Moreover, we show that diverse 2D materials such as graphene, BN nanosheets are applicable to this method and the materials obtained ranges from few layers to assembled macro-structures. These 2D-based materials can have good intrinsic elasticity and be used as highly flexible electrodes with further flexible structure design.



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## Unusual K-point Phonons in Noble Metal/Graphene Heterostructure

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Metal-graphene interface has been one of the most important subjects for fundamental science and device applications. Chemical bond formation of metal-graphene can be deduced from defect induced D-band and its second order mode, 2D band measured by Raman spectroscopy as a simple and non-destructive method. However, the mode located at  $\sim 1350 \text{ cm}^{-1}$ , which is normally known as defect induced D-band is intriguing for graphene deposited with noble metals (Ag, Au, Cu). The intensity ratio of mid-frequency mode at  $\sim 1350 \text{ cm}^{-1}$  over G-band ( $\sim 1590 \text{ cm}^{-1}$ ) exhibits not linear but resonant against laser wavelength. The frequency – laser energy dispersion is much less than conventional range,  $\sim 50\text{-}60 \text{ cm}^{-1}/\text{eV}$ . [1-2] This phonon modes of graphene at non zero phonon wave vector ( $q \neq 0$ ) around K points are activated by localized surface plasmon resonance, not by defects due to chemical bonds formation of metal-graphene. This is supported by density function theory (DFT) calculations on noble metals and Cr. In the point of metal-graphene interaction, contact resistances of graphene devices with Cu and Cr electrodes were compared with Raman results.

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# **Z2 monopole nodal lines and the Stiefel-Whitney insulator in the ABC graphdiyne**

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A striking consequence of nontrivial band topology is protected degeneracy of electronic energy bands. Examples vary from a surface Dirac point of a topological insulator to a Dirac point of graphene. Here, we study topologically protected band degeneracy occurring in a cousin material of graphene, dubbed graphdiyne [1]. Using first-principles calculations, we show that a three-dimensional ABC stack of graphdiyne hosts one-dimensional nodal ring in momentum space, which carries a  $Z_2$  monopole charge in the presence of inversion and time-reversal symmetry in the vanishing limit of weak spin-orbit coupling. Unlike the well-known nodal lines that carry the  $\pi$  Berry phase, the  $Z_2$  monopole nodal lines that occur in graphdiyne carry a Stiefel-Whitney number, which characterizes a two-dimensional parameter set of Hamiltonians on a sphere enclosing a nodal line. Based on the explicit calculation of a topological invariant, we also show that graphdiyne hosts a novel class of topological insulating phase referred to as a Stiefel-Whitney insulator under strain.

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## Coulomb drag behavior in graphene/MoS<sub>2</sub> heterointerface

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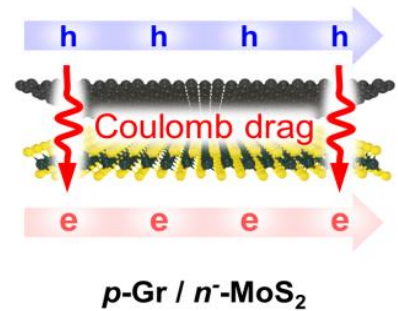
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Two-dimensional (2D) heterointerfaces often provide extraordinary carrier transport as exemplified by superconductivity or excitonic superfluidity [1, 2]. Recently, double-layer graphene separated by few-layered boron nitride demonstrated the Coulomb drag phenomenon: carriers in the active layer drag the carriers in the passive layer. Here, we propose a new switching device operating *via* Coulomb drag interaction at a graphene/MoS<sub>2</sub> (GM) heterointerface.

The ideal van der Waals distance allows strong coupling of the interlayer electron-hole pairs, whose recombination is largely suppressed by the vertical energy barrier at *p*-Gr/*n*-MoS<sub>2</sub> interface *via* dual-gate, whereas the lateral carrier transport is achieved *via* Coulomb drag. This device exhibits a high mobility (up to ~3,700 cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup>) even at room temperature, while maintaining a high on/off current ratio (~10<sup>8</sup>), outperforming those of individual layers. In the electron-electron drag regime, graphene-like Shubnikov-de Haas oscillations are observed at low temperatures. Our Coulomb drag transistor could provide a shortcut for the practical application of quantum-mechanical 2D heterostructures at room temperature.



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# Spin orbit engineered resonant second harmonic generation of artificially stacked Van der waal multilayers

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The non-centrosymmetric transitional metal dichalcogenides (TMDCs) and their heterostructures (HSs) provide a great platform for nonlinear optical (NLO) study, especially second harmonic generation (SHG). Different energy gaps TMDCs monolayers can be artificially stacked to enhance the SHG efficiency as well as broaden the spectral exciton resonance. In this study, we produced well aligned homo-bilayer, hetero-bilayer, and hetero-trilayer HSs, comprised of monolayer MoS<sub>2</sub> and its alloy MoS<sub>2x</sub>Se<sub>2(x-1)</sub>, and study their NLO properties. Photoluminescence analysis on all vertical HSs show clear A- and B-excitonic transitions from each constituent layer with no sign of interlayer transition, thereby confirming the excellent optical quality and isolated nature of each individual layer in the HS system. Broadband wavelength-dependent measurements on hetero-trilayer, using pico-second pulsed laser (spectral range:  $\lambda = 1100 \text{ nm} - 1600 \text{ nm}$ ) showed strong SHG signal in the spectral range of  $\sim 550 \text{ nm}$  to  $780 \text{ nm}$ . This essentially show that the SHG spectral response can be enhanced to a desired wavelength by controlling the Se concentration in MoS<sub>2x</sub>Se<sub>2(x-1)</sub> layer in the designed HSs system. The strengthening and widening effects are interpreted based on the SHG coupling between A- and B-excitons from the constituent layers. Our results demonstrate the feasibility of an artificial strong second-order susceptibility materials in broad spectral range by combining MoS<sub>2</sub> with different MoS<sub>2(1-x)</sub>Se<sub>2x</sub> alloys..

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# Simulation and study of the influence of the hole selective contact, buffer intrinsic layer, densities of interface defects, and transparent conductive oxide on TMO/c-Si heterojunction solar cell

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The influence of various parameters such as hole selective contacts (TMO), buffer intrinsic layers, densities of interface defects ( $D_{it}$ ), and then work function of transparent conductive oxide ( $\phi_{TCO}$ ) on TMO/c-Si solar cell performance was investigated using software simulation. Automat for the simulation of heterostructures (AFORS-HET) software was used for that purpose. Our results indicate that band bending, which is determined by the band offsets at the buffer intrinsic/c-Si and/or the TMO/c-Si heterointerface, could be critical to solar cell performance. The effect of band bending on solar cell performance and the dependence of cell performance on  $\phi_{TCO}$  were investigated in detail. Eventually, suggestive design parameters for high efficiency of  $\sim 27\%$  of TMO/c-Si solar cell fabrication are proposed.

**Keywords:** Transition metal oxide, hole selective contact, simulation, heterojunction solar cells

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# Two-terminal multibit optical memory via van der Waals heterostructure

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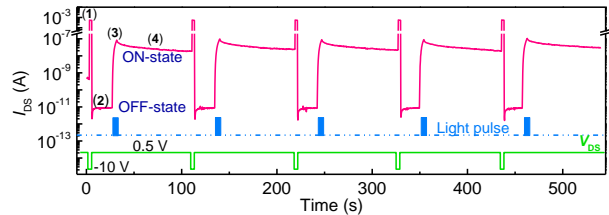
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Non-volatile optical memory devices based on van der Waals heterostructures (vdWs HSs) have recently gained significant interest as replacements for conventional silicon-based optical memory devices in image sensors, logic data processing, optoelectronic demodulators, and spectrum analysis systems. However, recently developed vdWs HSs-based optical memory devices rely on three-terminal configurations (gate, source, and drain), which limit the potential for device miniaturization and circuit integration. Moreover, high external programming voltages, high off-current, and high off-power consumption are typical challenges that must be solved for three-terminal memory devices [1, 2].

In this study, we propose a multilevel non-volatile optical memory device with a two-terminal floating-gate field-effect-transistor with MoS<sub>2</sub>/h-BN/graphene heterostructure. The current of the MoS<sub>2</sub> channel can be effectively switched between off- and on-states and retained for prolonged periods by a negative source-drain voltage ( $V_{DS}$ ) pulse and light pulse, respectively, as can be seen in the figure. The off-current is approximately  $10^{-11}$  A under -10 V of  $V_{DS}$  pulse, due to significant electron tunneling from the drain through the h-BN for storage in the bottom graphene floating gate, which eventually induces an effective negative gate bias to the MoS<sub>2</sub> channel. When exposing to a light pulse, the photo-generated holes in MoS<sub>2</sub> easily tunnel through h-BN to neutralize the stored electron in the bottom graphene layer owing to the small triangular hole-barrier of MoS<sub>2</sub>/h-BN. Thus, the device can be switched to the on-state ( $\sim 10^{-7}$  A). Moreover, our device exhibits a prolonged endurance over  $10^4$  programme-erase cycles, and a long retention time exceeding  $3.6 \times 10^4$  s. Furthermore, the high programming/erasing current ratio and long retention time of the MoS<sub>2</sub>/h-BN/graphene-based optical memory device provides a simple method to achieve multibit level optical data storage by light illumination. Under periodic light illumination of 18 light pulses, we successfully demonstrate 18 valid storage levels, corresponding to >4-bit for the prepared optical memory device.



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# Bandgap Renormalization in CsPbBr<sub>3</sub> Perovskite Quantum Dot/MoS<sub>2</sub> Heterostructure via Charge Transfer at Room Temperature

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Many-body effect due to mutual exchange and Coulomb interactions in electron-hole plasma decreases the intrinsic bandgap, producing bandgap renormalization [1,2]. Under external photoexcitation conditions, the strong charge Coulomb interaction in monolayer transition metal dichalcogenides is screened, leading to renormalization of electrical/optical bandgap, exciton binding energy and spin-orbit splitting.[3-5] The phenomenon, however, has been observed at low temperature and requires high photon excitation density. Here, we present bandgap renormalization at room temperature via charge transfer doping in a type-II heterostructure of MoS<sub>2</sub> monolayer and CsPbBr<sub>3</sub> perovskite quantum dots. The charge transfer doping through band bending at the heterostructure interface can be further enhanced by exciting CsPbBr<sub>3</sub> to produce a plasma screening effect in MoS<sub>2</sub>. This renormalizes the band structure of MoS<sub>2</sub>, causing redshifts of A and B exciton energy level by 82 and 78 meV respectively. The obtained bandgap renormalization is the highest value in MoS<sub>2</sub> achieved at room temperature. Our hybrid structure, which eliminates the need of high photoexcitation density dependence by efficient electron transfer from CsPbBr<sub>3</sub>, suggests possibilities in reducing the optical/electrical bandgaps in MoS<sub>2</sub> towards near infrared region. This will help realize practical devices incorporating TMDs for solar cell, photo-detector and LEDs.

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# Interplay of free charges of 2D van der Waals materials with the large polarization of ferroelectric oxides: a clue to photo-memristors

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Two-dimensional (2D) van der Waals (vdW) semiconductors can be integrated with functional materials and ferroelectric materials can be used to control charge distribution in 2D vdW semiconductors [1,2]. We can exploit polarization charge coupling effect in semiconductor-ferroelectric system and 2D vdW semiconductors can be used for this effect. We studied MoS<sub>2</sub> and WSe<sub>2</sub> layers on (111)-oriented ferroelectric PbTiO<sub>3</sub> (PTO) thin films, where the (111) triangular lattice is quasi-coherent with (001) 2D materials with respect to crystal orientation. Electrical response and transport characteristics were observed in 2D vdW-ferroelectric heterostructures by using conductive-atomic force microscopy. Enhanced resistive switching behavior was investigated in the heterostructures. The interactive relationship between free charges in 2D layers and ferroelectric polarization is important to obtain the polarization charge coupling effect. In particular, polarization states in the PTO thin films were a critical factor to control the transport characteristics. In addition, optical response was observed in the heterostructures. The optical response can be obtained because of the semiconducting properties of MoS<sub>2</sub> and WSe<sub>2</sub> layers. In addition to the semiconducting property, potential difference at the interface can also induce the separation of electron-hole pairs that yields photoresponse of the heterostructure. Therefore, ferroelectric polarization can behave as a physically doped electrode that gives enhanced optical response in the heterostructures. From these results, we can suggest a new platform of 2D vdW-ferroelectric system as a photovoltaic device by controlling conducting states with ferroelectric polarizations.

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## Enhanced Light–Matter Interactions in Self-Assembled Plasmonic Nanoparticles on 2D Semiconductors

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In this work, we report strong light–matter interactions in plasmonic Ag nanoparticles (NPs) hybridized on TMDs via an aging-based self-assembly process at room temperature. This hybridization is implemented by transferring MoS<sub>2</sub> monolayers grown via chemical vapor deposition onto thin-spacer-covered Ag films. After a few days of aging in a vacuum desiccator, the Ag atoms in the hetero-layered film diffused to the MoS<sub>2</sub> layers through a SiO<sub>2</sub> spacer and self-clustered onto MoS<sub>2</sub> point defects, resulting in the formation of Ag-NPs with an estimated diameter of ~50 nm. The photoluminescence intensities for the Ag-NP/MoS<sub>2</sub> hybrids were enhanced up to 35-fold compared with bare MoS<sub>2</sub> owing to the local field enhancement near the plasmonic Ag-NPs. The localized surface plasmon resonances modes of this hybrid were systematically investigated via numerical simulations and dark-field scattering microscopy. Our results introduce aging-based self-assembly methods for the plasmonic hybridization of TMDs.

## Ultra-short vertical-channel 2D transistors

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Ultra-short vertical-channel field effect transistors (VCFETs) based on two-dimensional (2D) semiconductors, with pre-patterned out-of-plane aligned source-insulating spacer-drain (SID) structure have been fabricated with a low-cost and complementary metal oxide semiconductor (CMOS)-compatible process. High-performance devices with channel length close to 10 nanometers (nm) were demonstrated with diverse 2D materials prepared by chemical vapor deposition (CVD) and mechanically exfoliation, respectively. As a typical example, the on-current of monolayer molybdenum disulfide (MoS<sub>2</sub>) grown by CVD technique can reach over 20  $\mu\text{A } \mu\text{m}^{-1}$  at bias voltage of 0.5 V, and another vital factor, the on/off ratio could be beyond 10<sup>8</sup>. Most importantly, the channel length could be simply controlled by the thickness of the atomically thin insulating spacer between source and drain electrodes, which is facile for device to be scaled down to several nanometers. This work provides a promising route toward the CMOS-compatible fabrication of ultra-scaled 2D semiconductor transistors.

# Tunable Negative Differential Resistance in van der Waals Heterostructures at Room Temperature by Tailoring Interface

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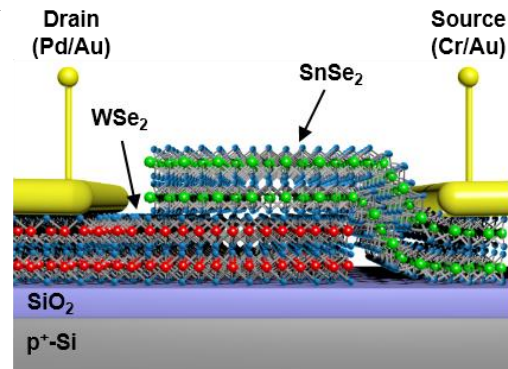
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**ABSTRACT:** Vertically stacked two-dimensional van der Waals (vdW) heterostructures, used to obtain homogeneity and band steepness at the interface, exhibit promising performance for band-to-band tunneling devices. Esaki tunnel diodes based on vdW heterostructures, however, yield poor current density and peak-to-valley ratios, inferior to those of three-dimensional materials. We for the first time to realize the NDR behavior in WSe<sub>2</sub>/SnSe<sub>2</sub> heterostructure system at room temperature and demonstrate that heterointerface control is key to achieving high device performance by constructing WSe<sub>2</sub>/SnSe<sub>2</sub> heterostructures in inert gas environments. While devices fabricated under ambient conditions showed poor device performance due to the observed oxidation layer at the interface, devices fabricated in inert gas environments exhibited extremely high peak current density up to 1460 mA/mm<sup>2</sup>, 3-4 orders of magnitude higher than reported vdW heterostructure-based tunnel diodes, with a peak-to-valley ratio over 4 at room temperature. Diode behavior can be further modulated by controlling the electrostatic doping and influenced by tunneling barrier as well.



**KEYWORDS:** Esaki diode, 2D tunneling heterojunction, negative differential resistance.



## Negative differential resistance in few-layer black phosphorus/SnSe<sub>2</sub> heterostructure

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Nowadays, ultimate device scaling of the conventional metal-oxide field-effect transistors (MOSFETs) together with lowered threshold voltage makes the subthreshold current problem more significant than that in long channel MOSFETs in terms of energy consumption. Recently, as an alternative of this conventional MOSFETs, tunneling field-effect transistors (TFETs) have received attention due to its potential low-power operation with smaller subthreshold swing. Also, it is known that the heterojunctions in TFETs are able to have higher device performance over homojunction-based TFETs because of those flexibility to form a steep band edge at the junction and select the channel material with higher carrier mobility. Two-dimensional (2D) van der Waals (vdW) materials are good candidates to overcome the typical lattice mismatch at the heterojunctions due to their absence of dangling bonds on the surfaces. Furthermore, diversity of heterostructures based on 2D vdW materials gives rise to high flexibility to engineer device properties of TFETs. Previously, BP-SnSe<sub>2</sub> heterostructure diode with the NDR behavior has been realized elsewhere, but only bulk form of the diode was developed at that time [1]. The point is that gate-tunable p-n heterojunction and band-to-band tunneling are the key to operate as TFET.

Here, we demonstrated black phosphorus-tin diselenide (BP-SnSe<sub>2</sub>) heterostructure tunneling field-effect transistors operating as both Esaki diode mode with negative differential resistance (NDR) region and backward diode mode at negative and positive gate bias, respectively. By introducing relatively high carrier concentration even in few-layer form of SnSe<sub>2</sub> sheets, only BP channel was able to be modulated by global electrostatic gating, making the device fabrication and operation much simpler. Gate-tunable type II staggered band alignment at the heterojunction was demonstrated by scanning photocurrent microscopy (SPCM). Temperature-dependent NDR behavior was unlikely with a conventional tunneling diode, but it was successfully explained by series resistance and thermal assisted tunneling mechanism. Also, the backward rectification behavior followed the thermionic emission theory, which confirmed that the another potential barrier had been created at the heterojunction due to the negative bias electrostatic gating. Besides, we pointed out that deposition conditions of the Al<sub>2</sub>O<sub>3</sub> passivation on the device were important to observe these effects.

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# Gate-tunable memory synaptic photomemristor based on two-dimensional transition metal di-chalcogenide

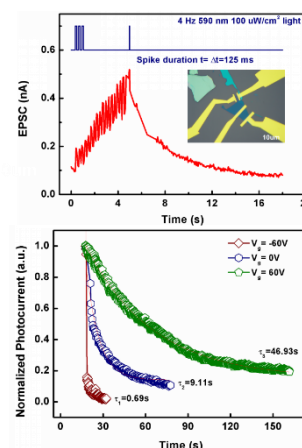
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Inspired by the biological neural system, artificial synapse will play an important role in artificial neural network beyond Von-neumann bottleneck [1-2]. As the combination of photodetector and synaptic transistor, synaptic photomemristor will be potentially applied in future electronic and optoelectronic fields [3-4].

In this work, mechanically exfoliated 3 layer MoS<sub>2</sub> was fabricated to a transistor with an on-off ratio over 10<sup>5</sup> as well as the mobility about 50 cm<sup>2</sup>/Vs. This device also shows high responsivity (over 8000 A/W) to monochromatic light from 365 nm to 850 nm. Afterwhile, a synaptic photomemristor based on MoS<sub>2</sub> phototransistor is design to mimic the retina and optic nerves via photonics stimulation mode. Photonic synapse functions containing short-term plasticity and long-term plasticity are simulated in the device. Particularly, we find that memory decay time is gate-tunable in MoS<sub>2</sub> synaptic photomemristor, where the decay time is respectively 0.69 s, 9.11 s and 46.93 s when applied gate voltage is -60 V, 0 V and 60 V. That means the memory and forgetting of the synaptic photomemristor can be controlled in device level which will be contributed to more powerful functions of the artificial synapse even artificial neural network.



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# Optical absorption enhancement in 2D MoS<sub>2</sub> monolayers: influences of interference and 3D dielectric material refractive index

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MoS<sub>2</sub>, a representative 2D semiconductor, has a sizable band gap leading to intensive research efforts for its optoelectronic device applications. However, limited optical absorption in atomically thin MoS<sub>2</sub> layers can be obstacles for high-efficiency light absorbing devices. To boost the optical absorption, researchers have used photonic nanostructures, Fabry-Perot-type cavities, and plasmonic metal nanostructures [1,2]. In this work, we investigate the optical properties of 2D MoS<sub>2</sub> that could be modulated by hybrid heterostructures consisting of 2D and 3D materials. Especially, MoS<sub>2</sub> monolayer on sub-100-nm-thick SiO<sub>2</sub>/Si substrates exhibit broadband omnidirectional absorption enhancement in the visible wavelength range [3]. Strong Raman peak intensity from the samples indicated the enhanced absorption, which could be attributed to the phase changes at the interfaces and those induced by the propagation of light in the SiO<sub>2</sub> layer. In addition, we prepared 2D MoS<sub>2</sub> monolayers conformally coated on Si and SiO<sub>2</sub> nancone (NC) arrays using metal organic chemical vapor deposition technique, and investigated the influences of the refractive indices of 3D NCs on the optical properties of 2D MoS<sub>2</sub> monolayers [4]. The photoluminescence and Raman intensities of the MoS<sub>2</sub> monolayer on the SiO<sub>2</sub> NC were higher than those on the Si NC, although the Si NC exhibited much lower optical reflectivity in the visible wavelength range compared with the SiO<sub>2</sub> NC. This work demonstrates that the 2D MoS<sub>2</sub> and 3D dielectric integrated structures can provide a useful means to manipulate the optical characteristics of the MoS<sub>2</sub> monolayers.

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# Near-Field Imaging of Charge Separation and Transfer at MoSe<sub>2</sub>-WSe<sub>2</sub> Lateral Heterojunction

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Two-dimensional transition metal dichalcogenides (TMDs) have enormous potential applications because they can be easily formed heterojunction (HJ) due to the weakly van der Waal's interaction. In particular, lateral TMDs HJ formed from two different monolayer TMDs have attracted for optoelectronic applications [1] because they form type-II band alignment, which lead to efficient charge carrier transfer and separation of electrons and holes.[2] However, because of spatial variation of exciton properties at HJ as well as having atomically sharp interface consequently need to nanoscale lateral spatial resolution, it is difficult to effectively investigate exciton characteristic at HJ. Here, we report the direct NF PL imaging of lateral MoSe<sub>2</sub>-WSe<sub>2</sub> HJ using near-field scanning microscopy (NSOM), which have lateral spatial resolution ~70 nm.[3] NF PL image find that PL quenching region exhibit across the HJ. This result reveal to depletion region due to charge separation. And also the depletion width is ~370 nm. In addition to, we show the efficient charge transfer at HJ region according to compare the ratio trion to exciton. The MoSe<sub>2</sub> and WSe<sub>2</sub> turn out effectively carry out n-type and p-type doping at depletion region.

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# Electrical characterization of graphene nanoribbon on h-BN

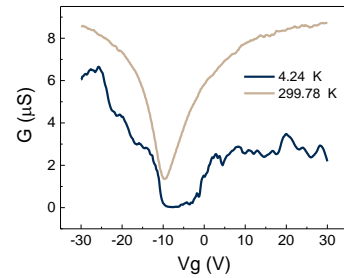
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Beneath huge interests on graphene in the last decade, forming an electronic band gap is still a challenge against its electronic logic-gate applications [1]. In this work we took advantage of quantum confinement to create an electronic band gap on graphene nanoribbons (GNRs) [2]. For the first time in our knowledge, a GNR field-effect transistor (FET) on a hexagonal boron nitride/SiO<sub>2</sub>/Si substrate was fabricated by a stencil mask technique where indium arsenide nanowire was used as a stencil mask. We performed the electrical measurement on the GNR FET for varying temperature between 300 K and 4.2 K. Diamond-like conductance patterns was observed on a conductance map obtained by sweeping source-drain and back-gate voltages at  $T = 4.2$  K, which indicates the existence of quantum dots on the channel [3]. The difference in electron- and hole-quantum dot's capacitances may reflect the presence of some extra charges in the GNR channel. The same conclusion was drawn by measuring and analyzing the competition behavior between the thermally-activated (TA) hopping and variable range hopping (VRH) electrical conductance phenomena, based on the conductance as a function of temperature at a given back-gate voltage (see right figure for two representative cases). Here, the characteristic temperature dividing the two regimes showed different puddle's height for electron- and hole-doped regions. In addition, the gate-voltage dependent behavior of the activation energy in the thermal hopping regime was also explained by the existence of localized negative charge on the channel.



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# RF Characterization and Modeling of Black Phosphorus MOSFETs

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Having a sizable bandgap and high carrier mobility, black phosphorus (BP) is a promising two-dimensional material for high-frequency electronic and optoelectronic devices. Further, for metal-oxide-semiconductor field-effect transistors (MOSFETs) operating at high frequencies, they must have a top gate of submicron length instead of the commonly used global back gate. However, without the global back gate to electrostatically induce doping in BP, top-gated submicron BP MOSFETs have not reached its full potential mainly due to large contact resistances. Here we report top-gated submicron BP MOSFETs with local contact bias electrodes to induce doping in the contact region. This resulted in orders-of-magnitude improvement in contact resistance ( $6 \text{ k}\Omega\cdot\mu\text{m}$ ) and, in turn, in current capacity ( $520 \text{ }\mu\text{A}/\mu\text{m}$ ) and peak transconductance ( $43 \text{ }\mu\text{S}/\mu\text{m}$ ). These improvements resulted in a forward current-gain cutoff frequency of 19 GHz and a maximum frequency of oscillation of 29 GHz, the highest reported for BP MOSFETs. The present approach could be extended to other 2D devices to reduce their contact resistance and to enhance their high-frequency performance.

The analysis shows also that with the contact bias, contact resistance is rendered to secondary importance and it is now the most important to increase transconductance  $g_m$  in order to have higher cutoff frequency  $f_T$  and maximum frequency of oscillation  $f_{MAX}$ .

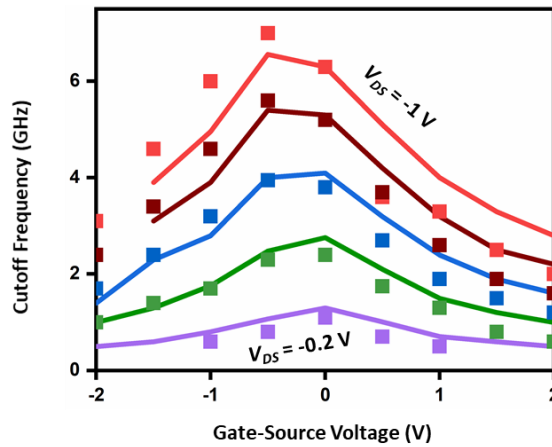
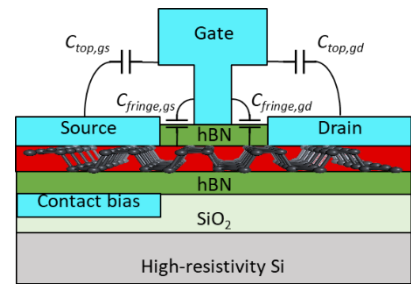


Fig.1 Modeled (solid line) and measured (square symbol) cutoff Frequency

# Bright light emission by suppressed exciton-exciton annihilation in monolayer WS<sub>2</sub> by laser irradiation

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Exciton transitions are mostly responsible for the optical properties of transition metal dichalcogenide monolayers (1L-TMDs). The important factor that determines the exciton emission of 2D semiconductors is exciton-exciton interaction. Specifically, exciton exciton annihilation (EEA) significantly limits the emission efficiency of 2D semiconductors.

Here, we observed reduced EEA rate in mechanically exfoliated monolayer tungsten disulfide (1L-WS<sub>2</sub>) by laser irradiation, causing improved light emission at the saturating optical pumping level. Time-resolved photoluminescence (PL) measurements showed that  $\gamma$  reduced from  $0.66 \pm 0.15$  cm<sup>2</sup>/s to  $0.20 \pm 0.05$  cm<sup>2</sup>/s simply using our laser irradiation. The shorter PL lifetime and lower PL and Raman intensity at low excitation levels suggested that laser irradiation increased the density of sulfur vacancies of 1L-WS<sub>2</sub>. Despite the number of defects increased in 1L-WS<sub>2</sub>, the induced defects cause suppression of EEA by hindering exciton diffusion. And I provide perspective on controlling EEA for maintaining high QY of 1L-TMDs even at high carrier density through for example by enhancing the simultaneous emission rate. Our results could provide an idea for high performance optoelectric devices.

# Edge introduced barrier in MoS<sub>2</sub>-WS<sub>2</sub> van der Waals heterojunctions

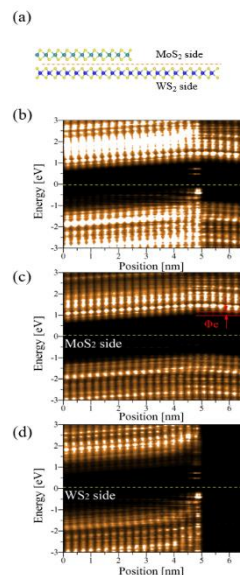
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Van der Waals structures based on two-dimensional transition metal dichalcogenides (TMDCs) open a great opportunity to develop next generation of electronic devices [1]. These van der Waals structures take advantage of its lack of dangling bond and effectively avoided the scattering caused by rough surface. But a typical configure of van der Waals homojunction or heterojunction is two monolayers partly overlapped with each other and left each one's edge unbonded [2]. Both experimental [3] and theoretical [4] researches have verified the existence and stability of metal terminal edges and dichalcogenide terminal edges in 2d TMDCs. It is interesting that how these non-passivated edges effect the transport properties in van der Waals structures. Here we present a numerical simulation on quantum transport of homojunctions composited by MoS<sub>2</sub> and WS<sub>2</sub> monolayers by implementing self-consistent density functional theory joint non-equilibrium green function (DFT-NEGF) [5] method. We find that due different types of edges (metal atom terminal or S atom terminal), the edge band bends downward or upward, as a result leading to a intralayer barrier in neighbor layer. The edge barriers can suppress electron carriers' transporting the heights of barriers can vary from a 80 meV to nearly 120 meV (depend on terminal atoms and Fermi level ). This suggest a new strategy to enhance the performance of van der Waals structures by edge passivation engineering and can be useful in designing photovoltaic photodetector or solar cells base on TMDCs or other 2D semiconductors.



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# Multifunctional reduced graphene oxide based electronic textiles for wearable electronic/optoelectronic applications

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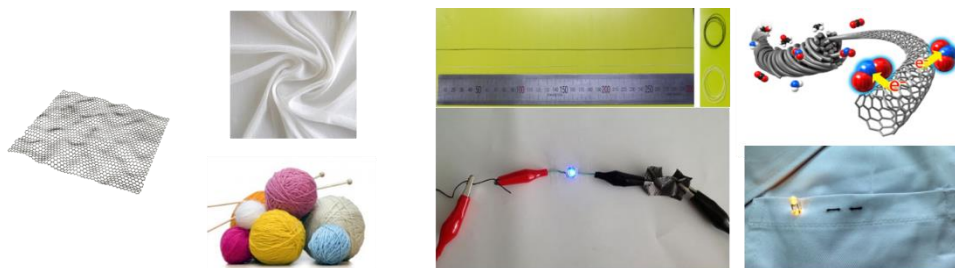
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Herein, we report the multifunctional graphene-based electronic textiles (e-textiles) composed of reduced graphene oxide (RGO) flakes and various textiles range from electrospun nanofibers to commercial yarns and fabrics. This method has the advantage of being applicable to the present textile industry because BSA and chemical leads to GO being easily attached to textiles that are widely used at present, e.g., cotton, polyester, and nylon. Interestingly, the RGO e-textiles exhibit a good electrical conductivity (greater than 100 S/cm) that is maintained under severe conditions, such as a large number of repetitive bending cycles (5000), and washing. Fully functional applications of wearable gas sensors in sensing harmful gases (i.e., NO<sub>2</sub>, NH<sub>3</sub>), ultraviolet detectors for 365 nm detection, fire sensors, etc. are demonstrated.[2] In addition, we fabricated the highly conductive and environmentally stable gold/graphene yarns with through a facile method by the electroless deposition of gold nanoparticles onto the surface of graphene yarns.[3]



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# Highly stretchable and biocompatible porous reduced graphene oxide films toward epidermal electronics

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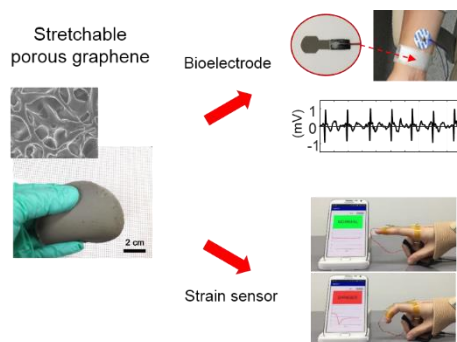
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Epidermal electronics have been extensively explored as an important platform for advanced wearable electronic applications. Wearable skin-like devices are typically fabricated using high-cost methods employing complex vacuum microfabrication processes, limiting their widespread potential in wearable electronics. Here, we present a low-cost, solution-based approach using electro-conductive reduced graphene oxide (RGO) flakes on elastic and porous poly(dimethylsiloxane) (PDMS) thin films for multifunctional, high-performance graphene-based epidermal bioelectrodes and strain sensors. These devices were fabricated employing simple coatings and direct patterning without using any high-cost and complicated micro-fabrication processes. The graphene bioelectrodes show a superior stretchability (up to 150% strain), with mechanical durability up to 5000 cycles of stretching and releasing, and low sheet resistance (1.5 k $\Omega$ /sq), and the graphene strain sensors exhibit a high sensitivity (a gauge factor of 7 to 173) with a wide sensing range (up to 40% strain). Fully functional applications of dry bioelectrodes in monitoring human electrophysiological signals (i.e., electrocardiogram (ECG), electroencephalography (EEG), and electromyogram (EMG)) and highly sensitive strain sensors for precise detection of large-scale human motions have been demonstrated.



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# Ferromagnetic Heavy Fermion System with Non-Fermi Liquid behavior in Antiperovskite $\text{Gd}_3\text{SnC}$

**Jongho Park**

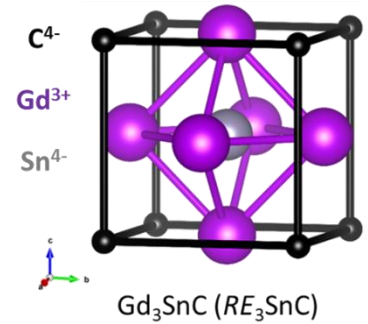
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Heavy fermions (HFs) are metallic compound and alloy typically originating from strongly correlated hybridization of f-electrons in materials. As a result of the strong hybridization between f-electrons, electrons exhibit  $\sim 1,000$  times larger effective mass than those from conventional metals, as being highlighted for the reason for the extraordinary phenomena such as unconventional superconductivity, quantum critical point (QCP; continuous phase transition at zero kelvin), and non-fermi liquid behavior (NFL; deviation of fermi liquid behavior in condensed matter). Up to date, most HFs appear from rare earth (Ce, Sm, and Yb) or actinide (U, Np, and Pu) compounds. However, Gd based HF systems are extremely rare due to the its strong localized electron nature of Gd  $4f^7$  electrons which are disadvantageous for composing the hybridization.<sup>1,2</sup>

Here, we report the new class of the Gd based HF material,  $\text{Gd}_3\text{SnC}$ , which possesses  $4f^7$  electrons in octahedral  $\text{Gd}^{3+}$  sublattice of antiperovskite, forming hybridization of f-electrons even in the Gd-based system. Phase transition at Curie temperature ( $T_C = 100$  K) is revealed from the electrical resistivity and magnetic moment measurements that confirming ferromagnetic ordering in  $\text{Gd}_3\text{SnC}$  below  $T_C$ .  $T^{1.5}$  dependence of  $C_P$  ( $C_P(\text{Gd}_3\text{SnC}) - C_P(\text{La}_3\text{SnC})$ ) strongly supports that ferromagnetic characteristics originated from  $4f$ -electrons in Gd atoms. Moreover, deviation of  $T^2$  below 21 K and logarithmic  $T$  dependence below 1 K in resistivity ( $\sim T^{1.1}$ ) and heat capacity, respectively, demonstrate NFL behaviors,<sup>2</sup> even in the ferromagnetic temperature regime. Finally, we establish that the gigantic sommerfeld coefficient ( $\sim 7,000$  mJ/mol  $\text{K}^2$ ) through the heat capacity measurement. According to the above results, We conclude that  $\text{Gd}_3\text{SnC}$  is ferromagnetic HF system with NFL behavior.



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## Energy Band Modulation to Improve HER Performance by Phase Selective Reduction of TiO<sub>2</sub>

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P25 is a well-known two-phase mixed TiO<sub>2</sub> with well-connected lattice structure between the anatase and rutile phases. This two-phase mixed structure has been reported as a high photocatalytic performance material by a number of papers due to the great photo-excited charge separation ability.[1] And the continuous reports of P25 have shown that this excellent charge separation performance of P25 is caused by low energy electron transfer process, despite the type-I heterojunction energy band structure between anatase and rutile phase which is easily induce charge recombination.[2,3]

In this study, we achieved great photocatalytic hydrogen evolution reaction (P-HER) performance with substantially low amount of Pt cocatalyst consumption by independent energy band modulation of anatase or rutile phase selectively in P25 through our phase selective reduction treatment of TiO<sub>2</sub>. The energy band structure of each TiO<sub>2</sub> phase in P25 was modulated to have a type-II heterojunction to improve charge separation ability because of the pristine P25 TiO<sub>2</sub> has type-I heterojunction. And we called the phase selectively reduced P25 TiO<sub>2</sub> as the OA/DR TiO<sub>2</sub> for ordered anatase/disordered rutile P25 and the DA/OR TiO<sub>2</sub> for disordered anatase/ordered rutile P25 samples. As a result, the OA/DR and DA/OR TiO<sub>2</sub> samples showed improved P-HER performance than pristine P25 TiO<sub>2</sub>. In particular, OA/DR TiO<sub>2</sub> showed significantly higher P-HER performance than other TiO<sub>2</sub> samples due to the low charge transfer resistance and type-II heterojunction energy band structure. In addition, OA/DR TiO<sub>2</sub> exhibited impressive P-HER performance with Pt cocatalyst which served as the active site of the hydrogen generation reaction and it is denoted as Pt-OA/DR TiO<sub>2</sub> as below. The Pt-OA/DR TiO<sub>2</sub> showed a higher rate of hydrogen generation under the simulated 1 sun light irradiation with only 10 times lower amount of Pt deposition than 0.5 wt % Pt deposited pristine P25. Consequently, we could conclude that the primary hindrance of P25 TiO<sub>2</sub> for P-HER was improper energy band structure between anatase and rutile phase and it should be overcome by energy band modulation of the phase-selective reduced phases.

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# Edge contact for Carrier Injection and Transport in MoS2 Field-Effect Transistor

**Ho Min Choi<sup>1</sup>, Jung Ho Kim<sup>2</sup>, Seok Joon Yoon<sup>2</sup>, Hamza Zad Gul<sup>2</sup>, Byoung Hee Moon<sup>1\*</sup> and Young Hee Lee<sup>1,2\*</sup>**

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Since the first monolayer MoS2 field-effect transistor (FET) was studied by Radisavljevic et al.,[1] the contact natures between MoS2 and metals have been studied extensively by many groups. Most of metal electrodes have been contacted with the channel from the top surface of MoS2, calling “top contact”, and its properties are well understood, but the physical property of the contact at the edge side of channel, calling “edge contact”, is still elusive. This edge contact was demonstrated to be very important for the graphene case because it decreases the contact resistance appreciably so that it can be usefully exploited in the structure of the vertical heterojunctions. In this poster, we present comparative studies between edge and top contact through various MoS2 thickness including monolayer, and various metals; i.e., Mn ( $\Phi_M = 4.1$  eV), Cr ( $\Phi_M = 4.5$  eV), and Au ( $\Phi_M = 5.1$  eV). Unlike top contacted MoS2 devices (TCMs) governed by “Fermi-level pinning” in earlier reports,[2] we observe that edge contacted MoS2 devices (ECMs) exhibit p-type, n-type and ambipolar type depending on the work function of metals and flake thickness. We also argue that the charge injection through the edge contact is dominated by the tunneling rather than thermionic emission based on the observations of negative Schottky barrier height and relatively small subthreshold slope. Our results not only give us a deep understanding of edge contact but also suggest that how useful it would be to employ edge-contact configuration to make high performance-MoS2 FET.

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# A high on/off ratio of top gate ZnO thin films transistors array with a buffer layer of self-assembled monolayer of molecule

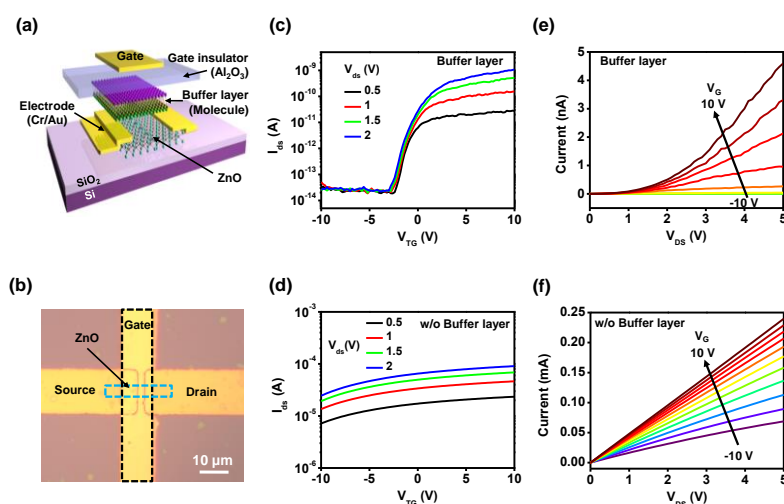
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We report the robust fabrication of top gate transistors arrays of semiconducting ZnO thin films with very thin buffer layer of self-assembly monolayer of molecule and aluminum oxide ( $\text{Al}_2\text{O}_3$ ) as top gate oxide. The ZnO thin film was growth by atomic layer deposition (ALD) method, which showed the surface defect-formation and limited to control the top gate devices.[1] In this study, we demonstrate a high on/off ratio of top gate field-effect transistors of ZnO thin film by using the buffer layer of self-assembled of monolayer molecule between ZnO film and  $\text{Al}_2\text{O}_3$  layer. Our devices showed 10,000 higher of on/off ratio compared to device without buffer layer. Using this new platform for logic circuit devices, we also demonstrated a large scale of inverter arrays with high device performance.



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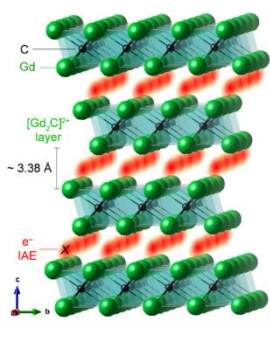
# Quasi-atomic electrons in two-dimensional ferromagnetic electride

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Electrides have emerged as exotic crystals, in which interstitial anionic electrons (IAEs) confined in positively charged cavities are responsible for the materials properties[1,2]. Here, we report that the IAEs in  $[\text{Gd}_2\text{C}]^{2+}\cdot 2\text{e}^-$  electride behave as ferromagnetic quasi-atoms in two-dimensional interlayer space and have their own magnetic moments of  $\sim 0.52$  Bohr magneton, inducing the ferromagnetism in  $[\text{Gd}_2\text{C}]^{2+}\cdot 2\text{e}^-$  electride. The substitution of paramagnetic chlorine atoms for IAEs proves the ferromagnetic IAEs with quasi-atomic nature from a clear transition to non-electride antiferromagnetic  $\text{Gd}_2\text{CCl}$  caused by attenuating exchange interactions of quasi-atomic IAEs with gadolinium atoms, consistent with theoretical calculations. These results confirm that quasi-atomic IAEs in two-dimensional interlayer space act as a single ferromagnetic element and trigger a ferromagnetic spin alignment within the antiferromagnetic  $[\text{Gd}_2\text{C}]^{2+}$  lattice framework. Our results open a new era to advance knowledge on quasi-atomic electrons that allow for exploring intriguing ferromagnetic materials



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## Noise nanospectroscopy as a probe for defect dynamics in monolayer MoS<sub>2</sub>

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The layered transition metal dichalcogenide (TMD) family of materials has been studied intensely for several years now, due their optical and electronic properties that make them promising candidates for next-generation electronics. More recently, structural defects that are present in these materials natively, or that are introduced during processing, have been recognized as a factor that strongly influences material properties, and both experimental work with probes such as TEM and STM, as well as theoretical work have studied the occurrence and electronic structure especially of point defects in TMD materials.

For the prototypical TMD material molybdenum disulfide (MoS<sub>2</sub>), both theoretical and experimental work has established that the by far most common defect is the sulfur monovacancy (V<sub>S</sub>). The presence of V<sub>S</sub> defects, in turn, has been linked to multiple anomalies observed in the electrical transport properties of monolayer MoS<sub>2</sub>: samples universally exhibit unexpectedly low mobilities, n-type characteristics, and large contact resistances regardless of contact metal work function. However, the mechanism underlying this link has remained unclear.

We use conductive-mode atomic force microscopy (c-AFM) to study charge switching phenomena in monolayer MoS<sub>2</sub>. Such switching processes, involving defects that possess multiple accessible charge states, can be detected by means of a spectral analysis of the noise current contribution. Due to the nanoscale dimension of the in-situ channel defined by the AFM tip size, we are able to probe only a few V<sub>S</sub> defects at a time. We find that V<sub>S</sub> defects exhibit switching between three distinct ionization configurations, corresponding to charge states 0, -1, and -2. The most probable charge configurations of these are 0 and -1. The high proportion of negatively charged V<sub>S</sub> defects suggests a plausible mechanism to explain the observed electrical transport anomalies of MoS<sub>2</sub> monolayers.



# Mobility engineering in the vertical field effect transistor based on van der Waals heterostructures

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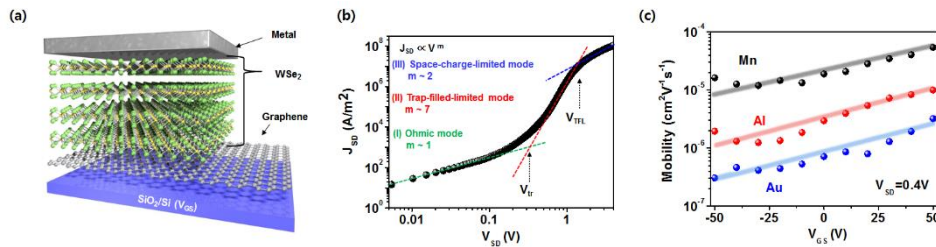
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Vertical integration of two-dimensional layered materials to form van der Waals heterostructures (vdWHs) offers new functional electronic and optoelectronic devices.[1,2] However, the mobility in vertical carrier transport in vdWHs of vertical field effect transistor (VFET) is not yet investigated in spite of the importance of mobility for the successful application of VFETs in integrated circuits (ICs).

In this work, we first investigated vertical carrier transport mechanism and the mobility in VFET of graphene/WSe<sub>2</sub> van der Waals heterostructures(Figure 1a).[3]The scattering by the traps in WSe<sub>2</sub> influenced the vertical mobility and three distinct transport mechanisms: Ohmic transport, trap-limited transport, and space-charge-limited transport.(Figure 1b) We also engineered the mobility in the VFETs under different drain biases, gate biases, and metal work functions. The Schottky barrier at the graphene/WSe<sub>2</sub> and metal/WSe<sub>2</sub> junctions decreased by applying a gate bias or reducing the metal work function, which could suppress the trap states by raising the Fermi level of WSe<sub>2</sub>. This suppression of the trap states in WSe<sub>2</sub> improved the vertical mobility in the VFET. In particular, the mobility in the VFET with Mn contact at +50 V gate voltage is about 76 times higher than the initial mobility of the VFET with Au contact.(Figure 1c)



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## Discovery of two-dimensional van der Waals Zintl phase and bidimensional polymorphism of ZnSb

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The discovery of new families of two-dimensional (2D) van der Waals (vdW) layered materials has always attracted great attention to pursue beyond graphene<sup>1-3</sup>. It has been challenging to artificially develop the vdW bonded layered structure that is constructed by the stacking of honeycomb atomic lattice composed of multi-components as in hexagonal boron nitride<sup>4</sup>. Here, through the dimensional manipulation of crystal structure, we create an unprecedented layer structured zinc antimonide, which is the 2D vdW Zintl phase of  $sp^2$ -hybridized honeycomb ZnSb lattice. It is verified from scanning tunneling electron microscopy and in-situ synchrotron X-ray diffractometry that the 2D vdW ZnSb has a stable and robust layered structure constructed by the vdW stacking of puckered honeycomb ZnSb layer and its overturned layer. This layered structure of 2D vdW ZnSb is evolved by the selective etching of lithium cations from the layered LiZnSb that is formulated by the alloying of lithium into  $sp^3$ -hybridized three-dimensional orthorhombic ZnSb lattice. The bidimensional polymorphism of ZnSb is only one example of a previously unnoticed phenomenon in Zintl phases at ambient pressure, which can be a common feature of TmPn (Tm : transition metal and Pn : Pnictogen) Zintl phases. This dimensional manipulation of crystal structure thus provides a rational design strategy to search for new 2D materials including Zintl and ionic compounds, enabling numerous combinations of chemical composition and corresponding physical properties.

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# Ferromagnetic two-dimensional van der Waals electride

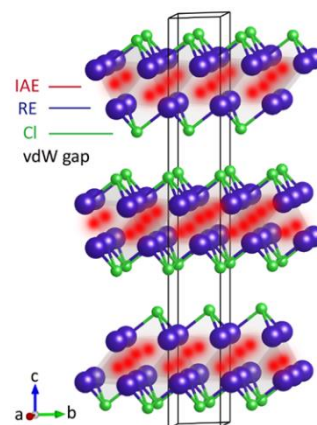
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Electrides are specific form of ionic crystals that contain interstitial anionic electrons (IAEs) serving as anions. IAEs occupying the structural cavities have been found as the form of solvated electrons in liquid or localized electrons in solid. Since the discovery of two-dimensional (2D) inorganic electride,  $[\text{Ca}_2\text{N}]^+\bullet\text{e}^-$  with 2D electron gas at interlayer space, various 2D inorganic electrides have been studied, which are distinguished by the localization degree of IAEs in 2D interlayer space.<sup>1</sup> Recently,  $[\text{Y}_2\text{C}]^{2+}\bullet 2\text{e}^-$  electride demonstrates anisotropic magnetism along the direction originated from spin-alignment of IAEs in 2D interlayer.<sup>2</sup>

Here, we report a new type of 2D electride with van der Waals layered structure with 2D electron gas at intralayer space. The experimental and theoretical investigation on the electrical and ferromagnetic properties of 2D van der Waals  $[\text{RECl}]^{2+}\bullet 2\text{e}^-$  (RE=Y and La) electrides will be discussed. Our findings provide an important insight into the design strategy of new 2D electrides with magnetism based on IAEs.



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## Application for High sensitive proximity sensor with CVD-growth MoS<sub>2</sub>

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In the present decade, two-dimensional materials, which has the layered structure bonded with Van der Waals force, have considered emerging materials for a long time. One of the widely known 2D material, MoS<sub>2</sub>, which is used for lubricants, has a semiconductor behavior, which has the band-gap from 2.8 eV with a monolayer to 1.0 eV with a bulk MoS<sub>2</sub>. A specific behavior, which a property changes with a different number of layers in 2D materials, have made these material utilize to various fields. For the optical proximity sensor, a light from the LED source has the infra-red region wavelength, which the absorption range of the sensor should be an infra-red region. A bulk MoS<sub>2</sub> has the band-gap around near IR region, which is around 1.2  $\mu\text{m}$ . In this study, we have demonstrated an application for an proximity sensor with CVD-growth MoS<sub>2</sub>. With the detecting behavior with the 811 nm light, the proximity sensor behavior like a resistance, which results the output voltage drops, connected with the amplifier output. We also makes the array to confirm the possibility for commercialize utilization.

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# Very High Open-Circuit Voltage in Dual-Gate Graphene/Silicon Heterojunction Solar Cells

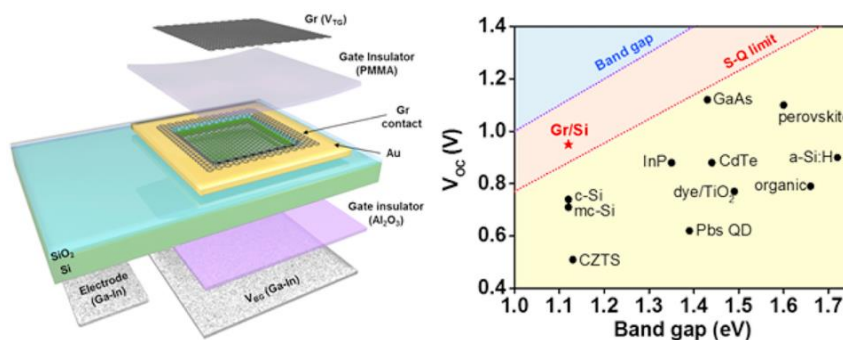
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Two dimensional (2D) layered materials and their heterojunctions with other materials are attracted because of their remarkable electrical and optical properties. In particular, graphene/semiconductor Schottky heterojunction is used for high performance solar cells. Here, we demonstrated very high open circuit voltage ( $V_{OC}$ ) in graphene/silicon heterojunction solar cell by dual-gate electric field application. The low density of states near Dirac point in graphene allows large modulation of graphene Fermi-level and corresponding Schottky barrier in a graphene/silicon junction. The top and bottom gate electric fields independently adjust the built in potentials of respective upper and lower silicon energy band to induce higher band bending (1.22 eV) than the bandgap (1.12 eV). As a result, a maximum  $V_{OC}$  of 0.94 V is achieved at the -8 V of top-gate voltage and 10 V of bottom-gate voltage, exceeding highest known  $V_{OC}$  for previous graphene/silicon solar cell ( $V_{OC} = 0.61$  V) and the S-Q Limit (0.84 V) of conventional silicon solar cell – a thermodynamic limit for the energy conversion efficiency of solar cells with a single band gap energy. The ratio of output power gain to input gate power ( $\Delta P_G/\Delta P_C$ ) is approximately  $10^{12} - 10^{14}$  with negligible power consumption in the gate ( $P_C = 1$  fW/cm<sup>2</sup> – 10 pW/cm<sup>2</sup>), resulting in the significant advances in the power generation ( $P_G = 40$  mW/cm<sup>2</sup>).



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# High responsivity, fast molybdenum disulfide photo-transistor using tunable schottky barrier

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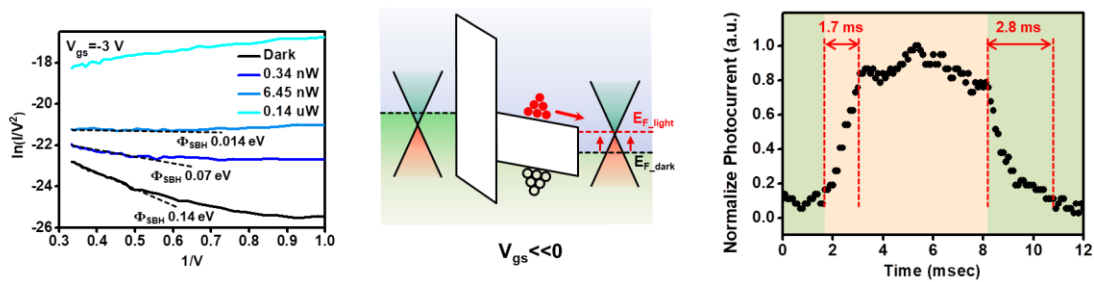
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Two-dimensional(2D) materials and their heterostructure are considered for future optoelectronic materials. In previous reports, Transition metal dichalcogenide(TMD) among 2D materials which is used for photodetector material shows high photo-responsivity up to  $10^3$  A/W. However, the photodetectors need long decay times in the range of several seconds or more.

We fabricated high responsivity, fast molybdenum disulfide(MoS<sub>2</sub>) photo-transistor using graphene-MoS<sub>2</sub> heterostructure. The graphene for source and drain has sub-30 nm gap to decreases the loss of carrier by recombination since carrier life time. A few-layer MoS<sub>2</sub> and h-BN for channel and dielectric layer are transferred by dry transfer method. We patterned CVD graphene for top-gate after graphene is transferred.

The gate bias generates the band bending which leads to transport excited carrier from MoS<sub>2</sub> to graphene. The transported carriers(electrons) pull fermi level up like N doping of graphene. The effect decreases schottky barrier height of graphene-MoS<sub>2</sub> junction.

It improves photo-transistor performance that the shorter channel length than diffusion length and schottky barrier modulation by excited carriers. The device has fast response time(<2.8 ms) and high photoresponsivity(> $2 \times 10^3$  A/W).



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# High performance graphene photodetector with van der Waals heterostructure through tuning carrier tunneling

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In the present decade, graphene, which is one of the large number of possible two-dimensional (2D) materials, is considered as a remarkable material for photonics and optoelectrics due to their specific properties such as gapless band structure which enables to modulate optical properties, ultra-fast carrier mobility which makes a fast modulation, a wide absorption ranges from ultra-violet (UV) to far-infrared (FIR), transparency and flexibility. However, a weak absorption properties and small built-in potential in a monolayer of carbon atoms have limited the properties such as an external quantum efficiency (EQE) range of  $\sim 0.1 - 1\%$  and a responsivity of a few of  $\text{mA W}^{-1}$ . Also, existing graphene-based photodetector with the lateral structure which has a photo response near graphene-metal junction is not an ideal for the harvesting efficient photons. To increase optoelectric properties in graphene, large number of devices integrating with other 2D transition metal dichalcogenides (TMDCs) materials and Quantum dots (QDs) materials which have high absorption properties were developed recently. However, integration with these materials limits the absorption range due to their own bandgap even graphene has advantages in large absorption range. Here, we developed large absorption range to infra-red (IR) range graphene photodetector with metal/insulator/graphene heterostructure by controlling the Schottky barrier. The absorption range can be controlled by utilize with different materials by controlling Schottky barrier. In visible range, we used Au/h-BN/graphene heterostructure which the existence of the h-BN tunneling layer makes extremely low dark current  $\sim 10^{-13}$  A. As the result, our photodetector has the high  $I_{\text{ph}}/I_{\text{dark}}$  over  $>20$  contrast to reported lateral graphene photodetector which has under 5. Finally, we also show the possibility of the IR photodetector with Ni/NiO/graphene heterostructure.

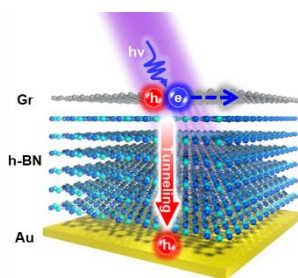


Fig 1. Schematic of Au/h-BN/graphene photodetector

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# Unveiling defect-related Raman mode of monolayer tungsten disulfide *via* tip-enhanced resonance Raman scattering

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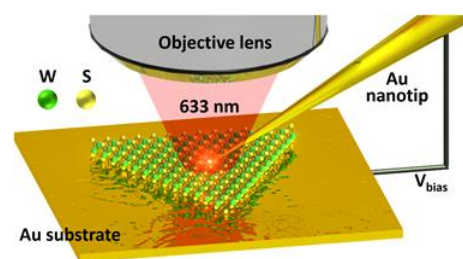
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Transition metal dichalcogenide (TMD) materials have been widely investigated because of unique electronic and optical properties. Among the monolayer TMD, a number of studies of tungsten disulfide (WS<sub>2</sub>) have been conducted because monolayer WS<sub>2</sub> has a relatively high photoluminescence quantum yield. According to these properties, the high-quality WS<sub>2</sub> are required to fabricate the device and an evaluation of sample quality is necessary by using the non-destructive technique like Raman spectroscopy. However, the conventional Raman spectroscopy has a limit to analyze nanoscale defects such as vacancies, substitutions, and grain boundaries which affect the electronic and optical properties of WS<sub>2</sub>. Therefore, the research using tip-enhanced Raman spectroscopy (TERS) called a nano-Raman technique is absolutely necessary to investigate the defects on nanometer scale for monolayer WS<sub>2</sub>.

In this study, we perform TERS experiments for the monolayer WS<sub>2</sub>. The high-resolution images of the TERS and scanning tunneling microscopy (STM) show TERS spectra depending on STM topography. We also demonstrate that the red-shifted A<sub>1g</sub> mode accompanied with the D and D' modes can be attributed to the defects in monolayer WS<sub>2</sub>. Furthermore, we identify that the emergence of new Raman modes can be induced by sulfur vacancies through the density functional theory calculations.



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## 2D Heterostructure for Enhanced Gas Barrier Performance via Synergetic Effect

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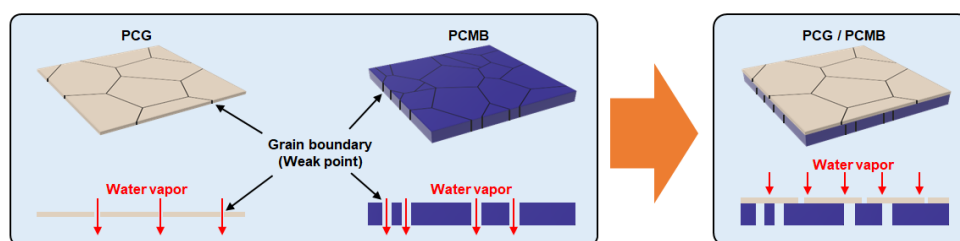
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Water is very harmful to organic light-emitting diode (OLED) compared to oxygen [1]. Therefore, the encapsulation of these devices with an impermeable gas barrier is necessary to ensure their long-term viability. Among the 2D materials, large-area monolayer graphene grown by CVD has been widely investigated as a gas barrier [2,3]. However, the gas barrier performance of graphene film is not as high as expected, due to the presence of structural defects such as grain boundaries and point defects in polycrystalline graphene (PCG) [4]. To improve the gas barrier performance, multi-stacked graphene films fabricated via a sequential transfer of PCG has been proposed [2]. However, while the performance of gas barrier, the transparency of the barrier increase, limiting to apply the transparent devices. In this study, we report on the dramatically enhanced gas barrier performance of polycrystalline monolayer graphene (PCG) film using a fabricated 2D heterostructure of a polycrystalline multilayered hBN (PCMB) film while maintaining a high optical transmittance of 96.2 % at 550 nm. The 2D heterostructure on a flexible PET film was fabricated via a sequence transfer of PCMB and PCG grown by CVD. The WVTR of individual PCG and PCMB films grown by CVD was 2.02 and 1.96 g/m<sup>2</sup>-day, respectively, which is a slight improvement compared to that of a bare PET substrate (2.16 g/m<sup>2</sup>-day) due to imperfections of their crystal structure. In sharp contrast, the 2D heterostructure that consisted of PCG on PCMB exhibited a WVTR value (0.07 g/m<sup>2</sup>-day) that was 30 times lower compared to that of the PET substrate. This is the lowest reported value among CVD-grown 2D materials. [5]



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# Highly Enhanced Photoresponsivity of Monolayer WSe<sub>2</sub> Photodetector with Nitrogen-doped Graphene Quantum Dots

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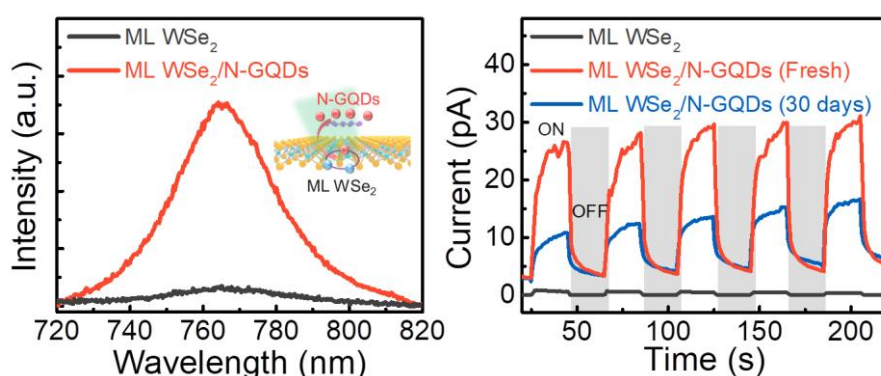
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Hybrid structures of two-dimensional (2D) materials and quantum dots (QDs) are particularly interesting in the field of nanoscale optoelectronic devices, because QDs are efficient light absorbers and can inject photocarriers into thin layers of 2D transition metal dichalcogenides (TMDs) which have high carrier mobility.

In this study, we present a heterostructure that consists of a monolayer of tungsten diselenide (ML WSe<sub>2</sub>) covered by nitrogen-doped graphene QDs (N-GQDs). The improved photoluminescence (PL) of ML WSe<sub>2</sub> is attributed to the dominant neutral exciton emission caused by the n-doping effect. Owing to strong light absorption and charge transfer from N-GQDs to ML WSe<sub>2</sub>, N-GQDs-covered ML WSe<sub>2</sub> showed up to 480% higher photoresponsivity than that of pristine ML WSe<sub>2</sub> photodetector. The hybrid photodetector exhibits good environmental stability, with 46% performance retention after 30 days under ambient conditions. The photogating effect also plays a key role in the improvement of hybrid photodetector performance. By applying the back-gate voltage modulation, the hybrid photodetector shows the responsivity of 2,578 AW<sup>-1</sup>, which is much higher than that of ML WSe<sub>2</sub>-based device.



## Thermal-driven electronic band change in layered semimetallic MoTe<sub>2</sub>

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Electronic, thermal and mechanical (structural) properties of layered transition metal dichalcogenides (TMDC) have shown non-trivial magnetoresistance and quantum states that are promising for next-generation electronics. In particular, unsaturated magnetoresistance and superconductivity have been demonstrated and explained by the exact compensation of electrons and holes in semimetallic MoTe<sub>2</sub>, which exhibits a significant temperature variation. Here, we clarify the origin of the temperature-induced non-trivial phenomena by investigating thermal expansion, band structure and phonon features of layered semimetallic MoTe<sub>2</sub>. The electron and hole concentrations were found to be largely correlated with the thermal expansion properties of the material along with the role of flexural phonon in the layered material with lattice distortion. Furthermore, resistivity characteristics of the semimetallic MoTe<sub>2</sub> show non-Fermi liquid behaviors.

## Layer-decoupling and stacking order modulation of multi-layered graphene by electrified-based electron injection

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Graphene has been extensively explored due to its promising intrinsic characteristics such as high mobility ( $200,000 \text{ cm}^2/\text{V}\cdot\text{s}$ ) and thermal conductivity ( $\sim 5000 \text{ W/m}\cdot\text{K}$ ), which inspired applications in nano-scale flexible and transparent electrical devices. Since graphene is a semimetal with negligible energy states at Dirac point, the Fermi level of graphene that affects its electrical performance can be largely modulated by (chemical) doping or electric gating. To realize the doping of electrons or holes in graphene, physical deposition of nitrogen, boron or hydrogen molecules on graphene or annealing the graphene with such gas molecules have been tried. However, these studies showed inevitable deformation of graphene lattices by a reaction with the molecules, creating defects, which could be observed as D peak in Raman spectrum. Other clean methods for an efficient doping of electrons (or holes) into graphene without defects have been demanded.

Here, we report an electron doping method without forming defects in multi-layered graphene by building an interface between two-dimensional electrified  $\text{Ca}_2\text{N}$  and graphene. The doping was confirmed by Raman spectroscopy that is sensitive to the change of the Fermi level of graphene and the formation of defects. The G and 2D Raman peak ratio and P1 and P2 components of 2D peak were dramatically changed after making a contact between graphene and the  $\text{Ca}_2\text{N}$ . We also discovered that the interaction between stacked graphene layers became weaker by the electron injection. Despite such efficient carrier injection, the D peak in Raman does not appear, which demonstrates our electron doping of graphene without making defects in graphene lattice.

# Ultraclean van der Waals heterostructure assembly with unity yield by solvent-assisted polydimethylsiloxane stamping

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Artificial van der Waals (vdW) heterostructures, restacked assemblies of two-dimensional vdW sheets, have received intense research interest due to the unique phenomena they exhibit, which often do not appear in the individual vdW materials [1, 2]. Typically, heterostructure fabrication involves vdW flake pickup, followed by deposition on the target sample. Early pioneering work on heterostructure assembly were based on coating vdW flakes with a polymer film such as PMMA or PLLA [2, 3, 4] followed by undercutting the flake via chemical removal of the substrate. More recent work has focused on reducing the organic contamination associated with the use of such polymers. The cleanest methods now available rely on dry pickup of vdW flakes, typically involving a stamp made of polydimethylsiloxane (PDMS) [5] which exploits the viscoelasticity of this material [6].

While PDMS-based dry flake pickup methods have enabled impressive advances, the approach suffers from a relatively low yield. Additionally, despite the improvement in sample cleanliness, reported heterostructures still do exhibit a marked degree of contamination, which typically manifests itself in the form of "bubbles". In this work, we present a PDMS-based, clean flake pickup technique that accomplishes bubble-free vdW heterostructures with a yield of unity. Like dry recipes, our method uses a PDMS stamp as carrier for vdW flakes, but it achieves its very high pickup yield by utilizing organic solvents to assist with pickup. We investigate the cleanliness afforded by our approach by exploiting the observation that hexagonal boron nitride (hBN) exhibits intense photoluminescence under green laser irradiation if in contact with organic contaminants [7]. We deliberately maximize the visibility of organic residues left behind in completed samples by fabricating hBN/hBN stacks with our technique, followed by an in-depth characterization that combines photoluminescence mapping with atomic force microscopic scanning.

Our findings confirm that in addition to its extremely high yield, our solvent-assisted heterostructure assembly approach can result in samples of unprecedented cleanliness. Furthermore, we demonstrate that our method is successful in transferring a wide variety of 2D vdW materials. As such, it represents a promising approach to address the limitations inherent to the heterostructure assembly techniques currently available.

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## Polymorphic 2D charge density waves in VTe<sub>2</sub>

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Layered transition metal chalcogenides (TMDs) have been extensively studied in terms of spontaneous lattice distortion such as charge density wave (CDW). In the layered crystals, new order parameters such as flake thickness, defect density and carrier density have been newly used to trigger CDW phase transition. While device applications require room temperature manipulation of the CDW, switching CDW in TMDs at room temperature remains a challenge.

We report vanadium ditelluride (VTe<sub>2</sub>) synthesized by flux method, which shows CDW transition at T=420 K. Since the transition temperature is above the temperature, a distorted lattice structure (monoclinic and C2/m) was observed in our VTe<sub>2</sub> at room temperature. Above the T=420 K, the lattice structure changes to a trigonal structure having a higher symmetry. We verified the CDW state by electrical transport measurement, powder and single crystal X-ray diffraction (XRD) and differential scanning calorimetry (DSC). The single-crystalline VTe<sub>2</sub> exhibits metallic transport characteristics at room temperature which is unique compared to other group 5 TMDs.

# Development of P-N diode in Few-layer ReS<sub>2</sub>/WSe<sub>2</sub> Stacking Structure

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<sup>1</sup>Hye Min Oh, <sup>1,2</sup>Mun Seok Jeong

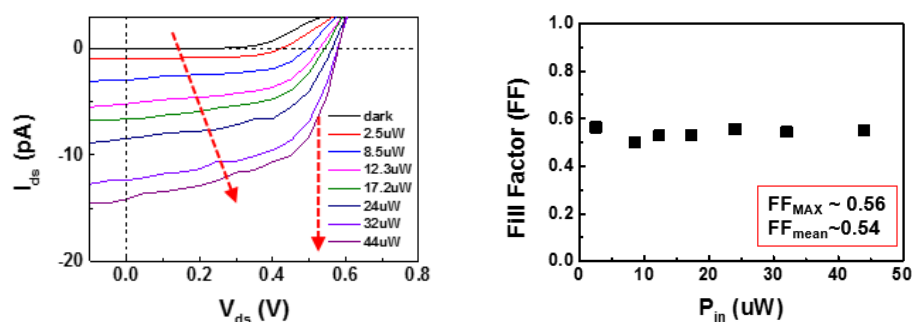
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Transition metal dichalcogenides (TMDCs) have attracted materials as a next-generation semiconductor because of the appropriate band gap, current on/off ratio and high mobility. Among them, ReS<sub>2</sub> has direct band gap not only monolayer but also bulk form. Also, it has a high photoresponsivity of 88,600 A/W[1]. Owing to these unique properties, ReS<sub>2</sub> can be a promising candidate for optoelectronic and electrical devices [1, 2].

This study presents the few-layer ReS<sub>2</sub>/WSe<sub>2</sub> heterostructure. Few-layer ReS<sub>2</sub> and WSe<sub>2</sub> were used to overcome the disadvantages of monolayer such as lack of absorbing layer and low opto-electric properties. We investigated photovoltaic effect, photocurrent, and also electrical properties. As a result, outstanding rectification behavior, fill factor and power conversion efficiency were obtained (Rectification ratio =  $7 \times 10^2$ ,  $FF_{\max} = 0.56$ ,  $PCE_{\max} = 1.5\%$ ). From these results, it is expected that ReS<sub>2</sub> will be a promising materials for flexible nanoelectronics [3].



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# Thickness-dependent Functionality of MoS<sub>2</sub>/MoTe<sub>2</sub> van der Waals Heterostructure

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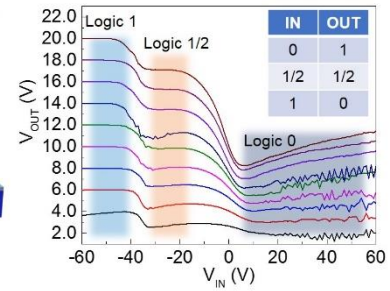
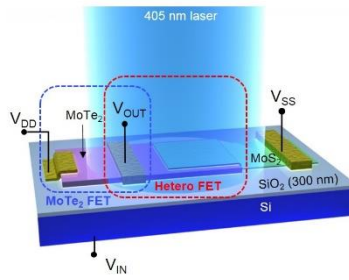
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Development of integration capacity of Si transistors is coined by the Moore's laws, i.e., the number of transistors in an integrated circuit (IC) doubles every 18 months. Continuation of Moore's law put an increasing demand on scaling down the lateral and vertical sizes of the transistor channels and challenge silicon-based technologies.

In the course of the development, recent atomically thin two-dimensional (2D) materials such as graphene (Gr), hexagonal boron nitride (hBN) and transition metal dichalcogenides (TMDs) provide the unprecedented platforms for building sub-microelectronics.<sup>[1][2]</sup>



We present various functional devices with a van der Waals heterostructure which are composed of molybdenum disulfide (MoS<sub>2</sub>) and molybdenum ditelluride (MoTe<sub>2</sub>). The device function can be modulated by changing the thickness of the MoTe<sub>2</sub> layer and the common gate bias. The device can perform the role of a p–n forward diode, backward diode, and Zener diode. In addition, we also utilized the available negative differential transconductance of the heterostructure to fabricate a multivalued logic device which exhibits three different logic states (i.e., a ternary inverter). Furthermore, our multivalued logic device can be transformed into a binary inverter by laser irradiation. This work provides a comprehensive understanding of the device fabrication and electronic device design utilizing thickness control.

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## All-optical logic devices via plasmon-exciton interconversion

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Nanophotonic devices manipulating light for high-speed computing are a counterpart of speed-limited electronic circuits. Although plasmonic circuits are a promising platform for subwavelength miniaturization, the logic-operation principle is still limited to mimicking those of photonic waveguides using phase shifts, polarization, interference, and resonance. Meanwhile, reconfigurable interconversion between exciton and plasmon engender emerging applications like exciton transistors and multiplexers, exciton amplifiers, chiral valleytronics, and nonlinear excitonics. Here, we propose all-optical logic gates realized by exciton-plasmon interconversion in Ag-nanowires (NW) overlapped on transition metal dichalcogenides (TMDs) monolayers. Excitons generated from TMDs couple to the Ag-NW plasmons, eventually collected as output signals at the Ag-NW end. Using two lasers, we demonstrate AND and OR gates by modulating single excitons in Ag-NW on MoS<sub>2</sub> and a half-adder by modulating dual excitons in lateral WSe<sub>2</sub> and WS<sub>2</sub>. Moreover, a 4-to-2 binary encoder is realized in partially overlapped MoSe<sub>2</sub> and MoS<sub>2</sub> using four-terminal laser inputs. Our results represent great advances in communication processing for all-optical photonics integrable with subwavelength architectures.

## Analysis of anomalous behavior at ferroelectric/two-dimensional material interface

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Ferroelectric materials have been considered as an emerging candidate in semiconductor industry due to the advantage for its nonvolatile property [1]. When ferroelectric material is employed as a gate dielectric for the field effect transistor (FET) of a two-dimensional (2D) material such as graphene, MoS<sub>2</sub>, and MoTe<sub>2</sub>, it is possible to induce a giant amount of carriers in the channel by polarization field of the ferroelectric and also show a nonvolatile memory operation. In many cases, however, the electrical coupling between 2D material and ferroelectric-oxide had shown abnormal behavior like anti-hysteresis which is opposite direction of ferroelectric polarization effect [2]-[5].

In our work, we fabricated dual gate FET that consists of ferroelectric/2D/hexagonal-BN (h-BN) structure, in order to distinguish ferroelectric polarization from charge trap by modulating both ferroelectric single crystal gate, PMN-PT (i.e. (1-x)Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>-PbTiO<sub>3</sub>) and normal gate, hexagonal BN. Through the electrical transport measurement in this structure, it is found out that the ferroelectric remnant polarization and trapped charges strongly interacts each other, and saturated polarization can overcome charge trap effect into the channel carrier which is reflected in the conductance of 2D channel.

The phenomena such as anti-hysteresis, current saturation behavior, on/off state, and hysteresis window change of channel current, will be discussed in terms of ferroelectric switching, polarization pinning, and the interface. To develop the 2D electronic system in ferroelectric nonvolatile memory device, those phenomena need to be studied in detail.

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## Significantly enhanced electromagnetic interference shielding effectiveness in graphene porous network with Fe<sub>3</sub>O<sub>4</sub> nanoparticles-intercalated 2D Ti<sub>3</sub>C<sub>2</sub> MXene

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The malfunction of electronic equipments and the threat of human health from electromagnetic (EM) waves radiated by electronic and telecommunication devices has attracted attention with the rapid development of information technology. Numerous electromagnetic interference (EMI) shielding materials have been developed to prevent unwanted EM radiations. The graphene with 3D foam-structure has been considered promising EMI shielding material due to its high conductivity and porous network structure leading to internal multi-reflection. However their shielding performance still needs further improvement for serving as commercial applications.

Herein, we demonstrate that the 3D porous graphene-based composites with Fe<sub>3</sub>O<sub>4</sub> nanoparticles-intercalated 2D Mxene (Ti<sub>3</sub>C<sub>2</sub>) flakes in a Poly dimethyl siloxane (PDMS) matrix lead to significantly enhance the EMI shielding effectiveness. This composite having a mechanical flexibility and lightweight exhibits a total EMI shielding effectiveness of 80 dB in a frequency range of 8.2-12.4 GHz (X-band). Beside contribution of magnetic loss component from Fe<sub>3</sub>O<sub>4</sub> nanoparticles, the superior EMI shielding performance results from the multiple reflections of the EM waves induced in the laminated structure of 2D layered Ti<sub>3</sub>C<sub>2</sub> as well as its high conductivity. Consequently, the brilliant EMI shielding performance of the composite opens the possibility to apply this material in various areas such as aerospace, military, and wearable/portable electronics.

## Graphene/PMN-PT field effect transistor with interdigitated electrode

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Recently, many grapheme-ferroelectric hybrid structures have been studied to investigate the possibility of candidate for potential memory device. Though hysteretic behavior of grapheme with ferroelectric gating can be qualitatively explained, a understanding of interface between grapheme and ferroelectric is still missing. Here, we analyzed transport properties of graphene and hysteresis loop of ferroelectric in each same devices. We fabricated interdigitated electrode (IDEs) on chemical vapor deposition grown grapheme film with various channel area with ferroelectric gating. Where we use PMN-PT ((1-x)Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub> single crystal as a ferroelectric material. Graphene film works as a channel for FETs as well as electrodes for ferroelectric thin film. The current is up to 20times different depending on the electrode configuration, hysteretic behavior is observed in the graphene channel consistent with the ferroelectric domain switching, and all devices with different graphene area have almost same hysteresis loop.

*Keywords: Interdigitated electrode, Graphene transistor, Graphene, Ferroelectric, PMN-PT*

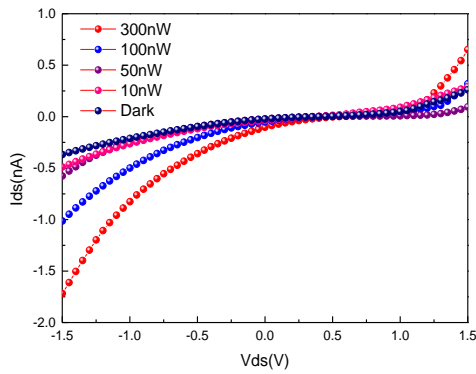
# A tunneling device for optoelectronic application with near-infrared light: Au/h-BN/MoTe<sub>2</sub> tunneling device study

**Geunwoo Hwang, Linfeng, Sun, Heejun Yang\***

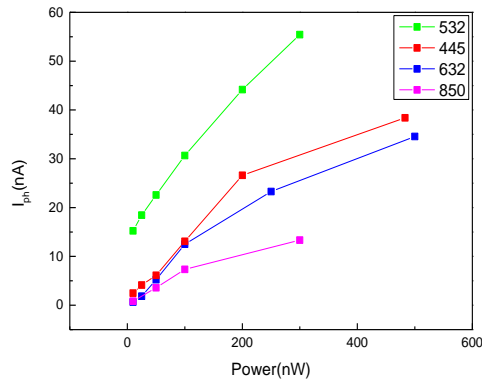
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2D materials with diverse band gaps are promising for opto-electronic applications, which attracts researchers for next-generation devices. Among many 2D semiconductors, MoTe<sub>2</sub> has a small bandgap of 1 eV, which is attractive for large photo-absorption. However, the on/off ratio between photo and dark current in MoTe<sub>2</sub>-based photo-detector is still high, particularly for its application in near-infrared light range; low dark current is required for applications. In this work, we conceived a tunneling junction to achieve a good on/off ratio ( $10^2$  at 445 nm) and a low dark current (0.5 nA at  $V_{ds}=1$  V). The different excitation wavelengths are used to characterize the tunneling device, which exhibits that our tunneling junction can be promising for sensitive wide-range photodetectors.



Fig(A)



Fig(B)

Fig (A) is Dark current and photocurrent at 850 nm light , Fig(B) is Photocurrent with different wavelengths.

## Hall magnetic sensor based on two-dimensional van der Waals materials

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A Hall magnetic sensor based on two-dimensional (2-D) van der Waals materials can make highly sensitive region with the help of good gate coupling from thin active channel where the mobile charges are accumulated and its high mobility. In this work, the Hall sensors having 2-D material channel is fabricated and the optimized condition for maximized sensitivity is estimated. A graphene Hall element shows well optimized property with high signal level from high carrier mobility above 3000 cm<sup>2</sup>/Vs and sensitivity of 2000 V/AT [1]. Then ionic gate system is employed for low voltage application and the optimized sensitivity of 3000 V/AT is achieved in 0.5 V bias near off state. Additionally, the analytical modeling for sensor performance prediction without magnetic field is suggested and proved in molybdenum disulfide (MoS<sub>2</sub>) Hall element [2].

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## Temperature-driven Lifshitz transition triggering non-Fermi liquid behavior in semimetal Nb<sub>2</sub>Se<sub>3</sub>

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Layered semimetals have attracted scientific interests to investigate intriguing physics such as topological insulating states, reversible structural phase transition, large magnetoresistance, superconductivity, and non-Fermi liquid behaviors. Such features mostly originate from their low dimensionality (2D geometry) combined with strong spin-orbit coupling and electron-electron interaction. In particular, Nb<sub>2</sub>Se<sub>3</sub> has been reported as a superconductor with its possible quasi one dimensional transport characteristics, resulting in an electrical anisotropy, but the interpretation of the results remains limited considering only electron carriers. Here, we have conducted systematic Hall measurements and magnetoresistance studies in monoclinic Nb<sub>2</sub>Se<sub>3</sub> single crystals at various temperatures. We discovered that the Nb<sub>2</sub>Se<sub>3</sub> shows a temperature-driven Lifshitz transition around 30 K. As temperature goes up, the material as a semimetal having both electron and hole carriers was changed into a hole dominant metallic system. Moreover, the temperature-resistance characteristics showed a non-Fermi liquid transport with the exponent value of 1.7 in the semimetallic phase below 30 K. We will discuss a putative origin of the non-Fermi liquid behavior based on the Fermi liquid model that is used for explaining the typical quadratic temperature dependency of resistivity in conventional metals.

# Continuous Thermopower from Capillary-induced Carbon Nanotube Yarn Thermoelectric Candle

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Harvesting energy from pre-existing energy reservoir is attractive technology. It can increase conversion efficiency of the system and moreover expand the accessibility of the electric devices at the extreme isolated environment by self-powering. Various types of harvester utilizing piezoelectric, triboelectric, thermoelectric effect have been suggested to achieve the practical amount of energy output for those purpose. Because the working principle of harvesters vary, they require unique and specific strategy to be applied for each of the circumstances. Here, we developed a new conceptual design of thermoelectric generator with Carbon nanotube yarn.

Candle consists of a paraffin and a cotton wick. And CNT yarn could work as a wick because of its porous structure characteristics which will induce capillary effect instead of the cotton yarn. But, not like the cotton, the CNT is conductive and known to have the thermoelectric effect with Seebeck coefficient  $\sim 80 \mu\text{V K}^{-1}$  [1]. Once the CNT yarn wick lighted, the fuel will be supplied continuously through the yarn to maintain a combustion and if the two end of the wick are wired, a measurable electrical potential will be shown between them. Even though the CNT yarn has small Seebeck coefficient, open circuit voltage  $\sim 40\text{mV}$  can be measured due to high temperature combustion process. To verify the robust thermoelectric energy harvesting properties, series and parallel connection of individual harvester were tested. This unique candle type energy harvester can open up the new application of CNT yarn for energy conversion field.



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# Charge trap effect at graphene channel caused by strong electrical affinity of fluorine

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Ever since graphene was discovered by mechanical exfoliation in 2004 [1], it has been a prospective material owing to its unique properties regarding quantum Hall effect, high mobility, transparency, and Young's modulus [2]-[4]. Nevertheless, graphene has been faced its limitations caused by zero band gap. Many studies have been undertaken to open the band gap by using strain, stacking geometry, intrinsic and extrinsic defect, chemical doping effect, *etc* [5].

Fluorinated graphene (FGr) is a promising candidate to solve the zero gap problem with its wide band gap and high thermal and chemical stability. Especially, its band gap is tunable with the carbon/fluorine ratio by gas fluorination, plasma fluorination, hydrothermal fluorination, and photochemical/electrochemical fluorination methods. Even though some results regarding opto/electronic nano-devices based on FGr have been reported previously [6]-[7], systematical study based on FGr with its device point of view is still lacking.

We have systematically studied electrical properties of both FGr/FGr and Gr/FGr devices by controlling electrical field, temperature, FGr/Gr ratio, and direction of fluorine group which is used as a dielectric material. We discuss here the phenomena of non-ohmic behavior and hysteresis by considering both the strong electron affinity of fluorine and the dipole moment of a carbon-fluorine covalent bond.

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# Plasma treatment induced n-type doping effect on few-layer WSe<sub>2</sub> field-effect transistors

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Transition metal dichalcogenides (TMDCs) with its two-dimensional layered structure have been considered as promising candidates to replace silicon-based electronic devices. To this end, however, significant improvements regarding large-area high quality material growth technique and other TMDC-customized device fabrication processes are still necessary. Since the standard doping techniques such as thermal diffusion and ion implantation are difficult to be directly applied with few-layer TMDCs due to its relatively thin body thickness, other TMDC-customized doping process should be extensively studied.

The TMDCs consist of a transition metal and two chalcogen atoms, and the structural defects such as chalcogen vacancies have been considered as the cause of unintentional doping. Plasma treatment technique with its simple and controllable feature has been suggested to efficiently control the structural defects in the TMDCs [1]-[5]. Herein, we report the n-doping effect of few-layer WSe<sub>2</sub> field-effect transistors (FETs) with controlled Ar plasma treatment. We have observed both the Raman peak shift and enhanced n-branch of the transfer characteristics in the few-layer WSe<sub>2</sub> FETs after the Ar plasma treatment, which are the sign of the n-type doping effect. Atomic force microscopy confirmed that the body thicknesses of the few-layer WSe<sub>2</sub> sheets showed no significant change after the Ar plasma. The n-type doping effect on the few-layer WSe<sub>2</sub> sheets induced by the Ar plasma could be explained by controlled creations of the Se vacancies in the WSe<sub>2</sub>. Note that M. Tosun *et al.* [5] reported the similar effect with hydrogen plasma treatment. We suggest that lateral p-n homojunction devices based on few-layer WSe<sub>2</sub> can be demonstrated with this simple plasma doping technique.

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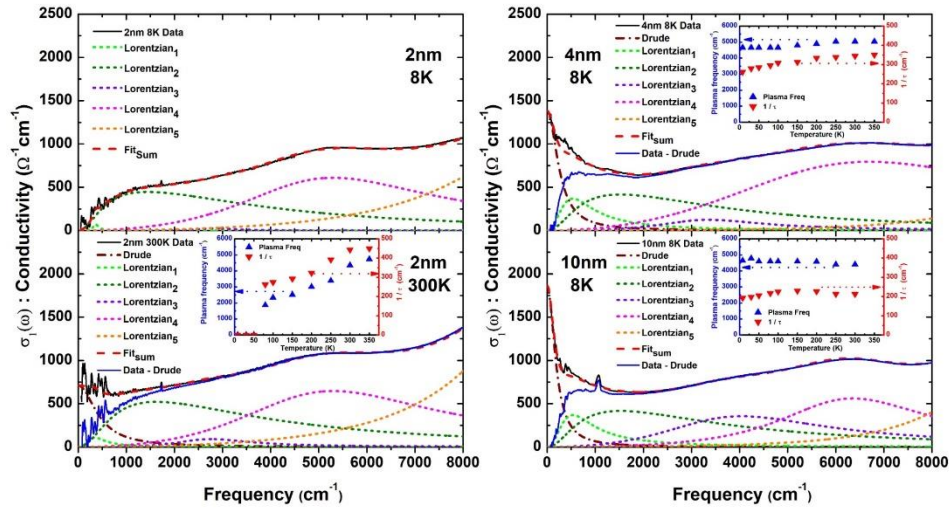
# Real Bandgap Investigation of CVD grown 1T'-MoTe<sub>2</sub> via Infra-red Spectroscopy

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Transition metal dichalcogenides (TMdCs) have attracted a massive attention due to their diverse properties ranging from insulator to metal and promising for wide applications, such as electronics, optoelectronics, photonics, and photovoltaics. Among these TMdCs, molybdenum ditelluride (MoTe<sub>2</sub>) has recently been of great interest owing to its extraordinary physical properties and structures. MoTe<sub>2</sub> has typically two polymorphs, including a stable semiconducting 2H phase and a metastable semimetallic 1T' phase. Many researchers are still studying about two polymorphs. Between those, we have investigated 1T'-MoTe<sub>2</sub> about optical properties via FTIR spectroscopy. 1T'-MoTe<sub>2</sub> film were prepared by CVD method from 10 nm to 2 nm. Then 1T'-MoTe<sub>2</sub> films were transferred on the undoped Si substrate and quartz substrate both for measuring Far-IR & Mid-IR (undoped Si) and Near-IR (quartz). Measurement was conducted under various temperature from 8 K to 350 K. From the measurement, we found the real bandgap of 1T'-MoTe<sub>2</sub> depending on thickness and temperature.



## Unusual quantum Hall effect across graphene grain-boundary grown by chemical vapor deposition

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We investigate the electrical transport properties at low temperature (2K) and high magnetic field (14T) of individual graphene grain boundary (GGB) which is formed when two grains merged during the growth. Graphene is synthesized using ambient chemical vapor deposition on polycrystalline Cu foil and the D band intensity of Raman mapping is used to detect GGB. Depending on angle alignment of GGB and induced radical dopants such as O and OH generated by UV treatment, We observed unusual quantum Hall effect (QHE) in which Hall resistivity ( $\rho_{xy}$ ) has the same oscillation peaks with longitudinal resistivity ( $\rho_{xx}$ ) at hole region while exhibiting the quantized value of QHE in single crystalline mono-layer graphene as seen in electron region. The property is reversed when the carrier type is changed in other device. We discuss this result, considering the effect of GGB and radical dopants to electrical transport properties of graphene leading to the coincidence of  $\rho_{xx}$  and  $\rho_{xy}$ .

## Thermal conductivity of Metal-Coated Carbon Fibers

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We measure the thermal conductivity of the metal-coated carbon fiber (MCF) with different metal thickness, using  $3\omega$  method [2]. In this method, the MCF is suspended in a closed cycle refrigerator. AC current at angular frequency  $\omega$  is applied to our sample to generate heat, and  $3\omega$  voltage resulting from the heat generation is measured. By analyzing  $3\omega$  voltage signal as a function of the angular frequency, the thermal conductivity ( $\kappa$ ) of MCF is estimated. The thermal conductivity of carbon fiber is measured 4.796[W/mK]. The thermal conductivity is increased to 24.18[W/mK] after metal coating on CF. We conclude that deposition of metal layer on the CF contributes an increase of thermal conductivity of CF. Our result demonstrates that thermal conductivity of CF is increased as metal thickness increased. Our result will assist in understanding the heat transport in cables and can be utilized to identify optimum thickness of metal for heat dissipation and conduction without compromising the electrical conductivity of metal coated carbon fiber.

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## Presence of Photothermal and Photoelectric in Partially Suspended PtSe<sub>2</sub>

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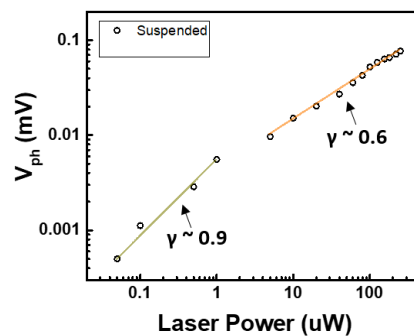
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We investigate the photoresponse of few layer PtSe<sub>2</sub>. The optically excited carriers in PtSe<sub>2</sub> dissipate their energy as heat to the phonon system or electrical current to electronic system. In order to understand the mechanism of how light energy is distributed inside PtSe<sub>2</sub>, we fabricate device in which PtSe<sub>2</sub> is partially suspended. Thus, our structure suppresses the heat conduction from flake to the substrate. We employed a custom built optical system for photocurrent measurement. Our system is equipped with a highly focused laser source with a spot size of ~1 $\mu$ m. We conduct photocurrent measurements by focusing the laser on the suspended area of the flake, using Keithley instruments and custom built labview program we are able to evaluate the photocurrent.

Analyzing the response of PtSe<sub>2</sub> depending on the laser power, we observe that, at low laser power, photovoltaic dominates, whereas, at high laser power, the nature of response changes to photothermal. We additionally demonstrate that the mechanism can also be controlled by the applied current, in low current region there is no heat generation even as laser power is increased however heat is only generated when the applied current is increased to few hundred nanoamperes. Our result concludes that heat generation in the sample is the principle due to which the nature of response changes. We perform temperature dependent resistance measurement through the result of this measurement, we are able to estimate the temperature rise in our sample. The sample temperature can increase few Kelvins. Our result shed light on the photoresponse mechanism of PtSe<sub>2</sub>, we are able to control the mechanism of photocurrent in our device by either the applied current or by varying the laser power. This will be helpful in advancing the art of light harvesting and photodetector applications.



## Broadband Photoresponse of Multi-layer MoS<sub>2</sub> from Ultraviolet to Infrared through Metal-Insulator Transition

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In this study, we fabricate few layer MoS<sub>2</sub> field-effect transistors on silicon nitride membrane. Through dry transfer technique we stacked hBN (dielectric) and graphene (top gate) on our MoS<sub>2</sub> channel. We used a closed cycle refrigeration system to investigate the electrical properties of our device and observed MIT behavior on the high positive gate bias. This is also confirmed by measuring resistance as a function of temperature. We utilized custom built optical measurement system with a high resolution focused laser beam to characterize the optical response from our device. Our device shows considerable photocurrent as the gate bias is changed from negative to positive, however at high positive gate bias our sample shows metallic transition which eliminates photocurrent in the channel. We irradiate the sample with 9.6um infrared (IR) source and observe the sample resistance remains unchanged until our device transition to the metallic state. The sample resistance shows a significant change which we attribute to heat generation by the IR source. We have demonstrated a switchable room temperature visible to the IR detector on multilayer MoS<sub>2</sub> using MIT. Through our work we aim to identify the mechanism. Our result are a significant achievement towards a commercially viable photodetector using MoS<sub>2</sub> such as touch sensor panels, image sensors and communication devices.

## The broad range pressure detection by electro-thermal response of metal-coated carbon fiber

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In this study, we examined the temperature dependence of metal-coated carbon fiber (MCF) on Argon (Ar) environment by making a few hundred metal layers on the surface of carbon fiber which is about 7 $\mu$ m in diameter. Temperature of MCF was increased up to 350K when the current was applied due to Joule heating effect. Such a pressure-dependent temperature of MCF indicates that the heat loss mechanism is governed by the convection via Ar gases. Currently, detection limit is around 10<sup>-4</sup> (torr) in a low vacuum gauge by using a gold-plated tungsten wire. However, our results show that the electron-thermal detection of the pressure is in range of 10<sup>-3</sup> (torr) to 10<sup>-8</sup> (torr). The higher aspect ratio of the length to the diameter, larger than 1000, and the low thermal conductivity of MCF because the heat to be taken away by the interaction with Ar gases, rather than to be lost by the conduction along the MCF. Furthermore, the electro-thermal response of MCF is feasible at low electric power (less than 100 $\mu$ W). Our results pave the way for detecting the high vacuum level by using convectional heat loss.



## Transport characteristics of van der Waals junction assembled with NbSe<sub>2</sub> and FeSe

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Josephson effect and Andreev reflection are novel quantum phenomena which are observed only at the boundary of superconductor(S.C.). Recently, van der Waals junction[1-3] provide the new kind of interface between S.C. and the other materials, such as S.C., insulator, metal, semiconductor and magnetic materials. Using high quality single crystal  $\beta$ -FeSe[4], NbSe<sub>2</sub> and the well-known dry transfer technique widely applicate in van der Waals materials, we fabricated the vertically stacked S.C./S.C. van der Waals junction. In this poster, we present the results of transport and interface characteristics of the van der Waals junction assembled with two different superconductors.

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## Electronic and optical properties of staggered ZnO/ZnO<sub>1-x</sub>S<sub>x</sub>-ZnO<sub>1-y</sub>S<sub>y</sub>/ZnO quantum well for bluish-green light-emitting diodes

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The design of staggered ZnO/ZnO<sub>1-x</sub>S<sub>x</sub>-ZnO<sub>1-y</sub>S<sub>y</sub>/ZnO ( $x > y$ ) quantum-well (QW) leads to significant have much larger spontaneous emission with improvement in electron-hole wave function overlap and spontaneous emission as compared to that of the conventional ZnO<sub>1-x</sub>S<sub>x</sub>/ZnO QW. Staggered QW structures are studied to eliminate the influence of polarization-induced electrostatic field upon the optical performance of light-emitting diodes (LEDs). Optical properties of staggered ZnO/ZnO<sub>1-x</sub>S<sub>x</sub>-ZnO<sub>1-y</sub>S<sub>y</sub>/ZnO ( $x > y$ ) QW LEDs are theoretically investigated and compared by using the multiband effective mass theory. These results are compared with those of conventional ZnO<sub>1-x</sub>S<sub>x</sub>/ZnO QW structures. As simulation results, the best optical characteristics are obtained for the staggered QW LEDs. Staggered QW structure has much larger matrix element than a conventional QW structure because spatial separation is substantially reduced between electron and hole wave functions with the inclusion of a staggered ZnOS layer. Superiority of this novel design relies on the strength of its enhanced overlap between electron and hole wave functions, hole's uniform distribution and suppression of electron leakage in the LED device. The analysis indicates the potential of using staggered QW concept in ZnO-based bluish-green LEDs. In this work, using the APSYS (abbreviation of advanced physical models of semiconductor devices) 48 simulation program, various staggered QW LEDs are theoretically studied in detail by performing computational simulations [1,2]. Critical physical mechanisms and the proper designs of staggered-QW bluish-green LEDs were examined which are lying behind the improvement of the optical performance.

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# Anion-Cation Double Substitution in Transition Metal Dichalcogenide to Accelerate Water Dissociation Kinetic for Electrocatalysis

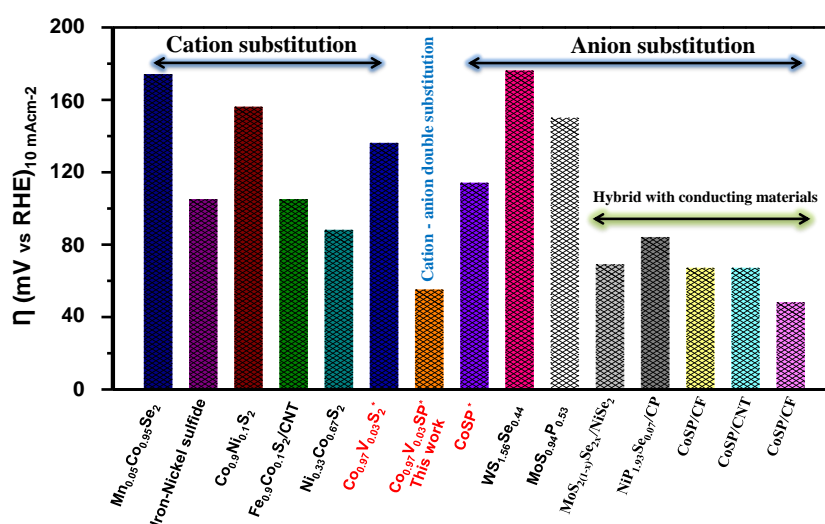
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Until now, many works have shown that the hydrogen evolution reaction (HER) performance can be improved by anion or cation substitution into the crystal lattice of pyrite-structure materials. However, the synergistic effects of anion-cation double substitution for overall enhancement of the catalyst activity remains questionable. Here, the simultaneous incorporation of vanadium and phosphorus into the CoS<sub>2</sub> moiety for preparing 3D mesoporous cubic pyrite-metal Co<sub>1-x</sub>V<sub>x</sub>SP is presented. It is demonstrated that the higher catalytic activity of CoS<sub>2</sub> after V incorporation can be primarily attributed to abundance active sites, whereas P substitution is responsible for improving HER kinetics and intrinsic catalyst. Interestingly, due to the synergistic effect of P–V double substitution, the 3D Co<sub>1-x</sub>V<sub>x</sub>SP shows superior electrocatalysis toward the HER with a very small overpotential of 55 mV at 10 mA cm<sup>-2</sup>, a small Tafel slope of 50 mV dec<sup>-1</sup>, and a high turnover frequency of 0.45 H<sub>2</sub> s<sup>-1</sup> at 10 mA cm<sup>-2</sup>, which is very close to commercial 20% Pt/C. Density functional theory calculation reveals that the superior catalytic activity of the 3D Co<sub>1-x</sub>V<sub>x</sub>SP is contributed by the reduced kinetic energy barrier of rate-determining HER step as well as the promotion of the desorption H<sub>2</sub> gas process.



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# Augmented Quantum Yield of a 2D Monolayer Photodetector by Surface Plasmon Coupling

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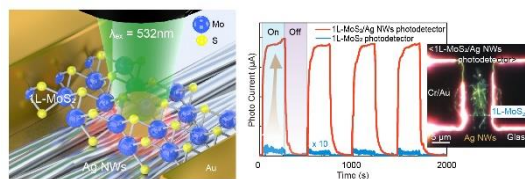
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Since discovery of direct band gap and broad absorption range from UV to IR regions at monolayer [1], transition metal dichalcogenides (TMDCs) such as MoS<sub>2</sub>, WS<sub>2</sub> and WSe<sub>2</sub> are regarded as promising materials in nano-scale optoelectronic devices. However, 1L-MoS<sub>2</sub> is difficult to applicate for practical optoelectronic devices such as photodetector, solar cell and light emitting diode due to an extremely low optical quantum yield (QY) [1]. To enhance the optical QY of 1L-MoS<sub>2</sub>, the prospective method with the surface plasmon (SP) effect have been utilized using metal nanostructure [2]. In this investigation, a high-gain 1L-MoS<sub>2</sub> photodetector was successfully realized, based on the SP effect of the Ag NW network. Through systematic optical characterization of the hybrid structure consisting of a 1L-MoS<sub>2</sub> and the Ag NW network, it was determined that a strong SP and strain relaxation effect influenced a greatly enhanced optical QY. The PL emission was drastically increased by a factor of 560, and the main peak was shifted to the neutral exciton of 1L-MoS<sub>2</sub>. Consequently, the overall photocurrent of the hybrid 1L-MoS<sub>2</sub> photodetector was observed to be 250 times better than that of the pristine 1L-MoS<sub>2</sub> photodetector. In addition, the photoresponsivity and photodetectivity of the hybrid photodetector were effectively improved by a factor of ~1000. This study provides a new approach for realizing highly efficient optoelectronic devices based on TMDCs.



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## Organometal Halide Perovskite to Optoelectronic Devices Fabricated with Homogeneous Nano-seed.

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The lack of methods for tailoring directional growth of perovskite films has limited the full potential for perovskite films in many applications. Herein, we present a new design methodology capable of freely tailoring the directional growth of methylammonium lead bromide (MAPbBr<sub>3</sub>) films between (100) and (111) directions. It is found that nucleation or seeding of organometal halide perovskites critically determined the crystal orientation and influenced defects and morphology of perovskite films. MAPbBr<sub>3</sub> quantum dots (QDs) behave as the point of seeding to crystallization. The growth of (100) direction is induced to (111) direction via the two ligands exchanges of dimethylsulfoxide (DMSO) with the ligands (oleylamine, oleic acid) and MA<sup>+</sup>. These mechanisms produce the (100) and (111)-oriented MAPbBr<sub>3</sub> film, which can control the distribution of plane by the seed concentration. The (111)-oriented MAPbBr<sub>3</sub> films formed by seeds were achieved that is improved photoluminescence (PL), uniform luminescence, higher stability, enhanced photocurrent and less surface defect than (100)-oriented MAPbBr<sub>3</sub>. In particular, we suggest that (111) oriented MAPbBr<sub>3</sub> films have strong direct bandgap properties and (100) oriented MAPbBr<sub>3</sub> films have slightly indirect bandgap properties, according to our results.

# High peak-to-valley Current Ratio in SnSe<sub>2</sub>/MoTe<sub>2</sub> tunnel diode

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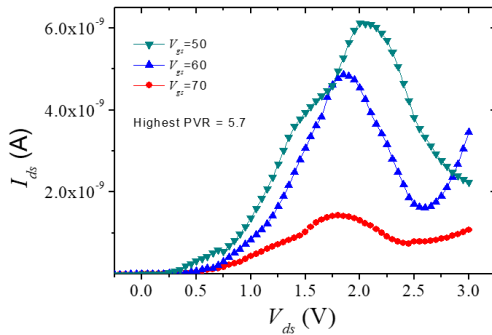
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Recently, the band-to-band tunneling devices based on Transition Metal dichalcogenides (TMDs) van der Waals (vdW) heterostructure attract a great attention due to its flexibility and various unique electronic properties[1]. In the tunneling diode with TMD, low peak-to-valley current ratio is a main issue which should be solved for high performance[2].

Here, we fabricated a tunneling diode composed of high-electron mobility SnSe<sub>2</sub> and narrow-band gap MoTe<sub>2</sub> vdW heterostructure. We deposited metal contact at the bottom of TMDCs for reduce the effect of Fermi level pinning. In our structure, the peak-to-valley current ratio is about 5.7, which is the highest value in TMDs-based devices.



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## 2-D Transition Metal Dichalcogenides Charge Transport Layers for Perovskite Solar Cells

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Perovskite materials have attracted much attention in solar cell studies, due to their attractive properties such as high charge mobility, long carrier diffusion lengths and low trap density. Despite these advantages, perovskite solar cells (PSCs) suffer from the instability of device performance. Perovskite materials undergo rapid degradation in ambient conditions. The PSCs cannot maintain its initial performance without any passivation. Although many studies have been carried out to solve this instability, this is still remained inevitable issue for commercialization of PSCs.

Generally, the PSCs is composed of transparent conductive oxides (TCO), electron and hole transport layer, perovskite layer, and electrode. The materials used in PSCs and their interfaces are important for device performance and stability. In particular, the electron and hole transport layers directly contact with perovskite layer, they can play an important role in PSCs. Some materials such as PEDOT:PSS and Spiro-OMeTAD are conventionally used as charge transport layers. However, due to their hygroscopic and acidic properties, they internally accelerate the degradation process in PSCs. To prevent this internal degradation, other stable materials are required. Here, we suggest transition metal dichalcogenides (TMDs) as inorganic charge transport materials for stable PSCs and will discuss charge transporting mechanisms of TMDs-based PSCs.

# Highly sensitive graphene biosensor by monomolecular self-assembly of receptors on graphene surface

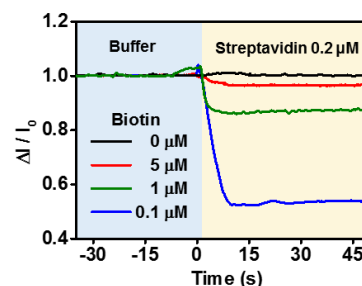
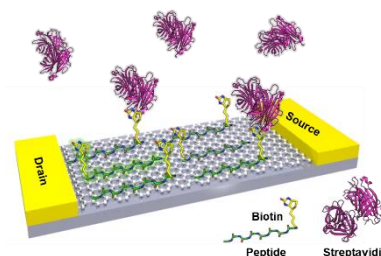
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Graphene has attracted a great deal of interest for applications in bio-sensing devices because of its ultra-thin structure, which enables strong electrostatic coupling with target molecules and its excellent electrical mobility promising for ultra-fast sensing speeds. However, thickly stacked receptors on the graphene's surface interrupts electrostatic coupling between graphene and charged biomolecules, which can reduce the sensitivity of graphene biosensors. Here, we report a highly sensitive graphene biosensor by monomolecular self-assembly of newly designed peptide protein receptors. The graphene channel was non-covalently functionalized using peptide protein via the  $\pi$ - $\pi$  interaction along graphene's Bravais lattice, allowing ultra-thin monomolecular self-assembly through graphene lattice. In thickness, dependent characterization, a graphene sensor with a monomolecular receptor (thickness less than 1 nm) showed five times higher sensitivity and three times higher voltage shifts than graphene sensors with thick receptor stacks (thicknesses greater than 20 nm), which is attributed to excellent gate coupling between graphene and streptavidin via an ultrathin receptor insulator. In addition to having a fast-inherent response time (less than 0.6 s) based on extremely high carrier mobility in graphene, our graphene biosensor is a promising new platform for highly sensitive real-time monitoring of biomolecules with high spatiotemporal resolution.



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## **SWCNT/h-BN heterostructures: fabrication, interface and transport properties**

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*Abstract will be updated soon..*

# Coexistence of indirect- and direct-bandgap excitons in monolayer WSe<sub>2</sub>

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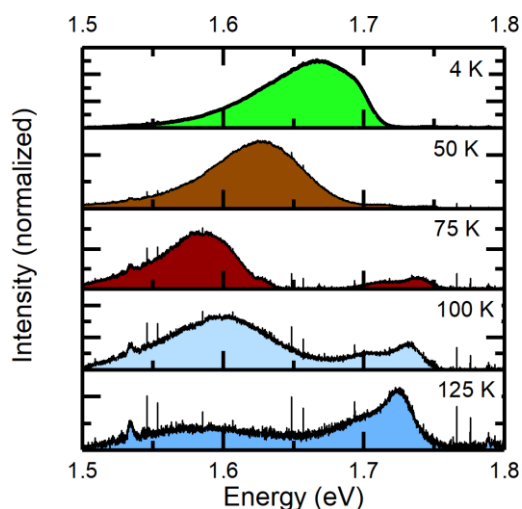
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Group VI transition metal dichalcogenides (TMDs) with chemical formula MX<sub>2</sub> (M=Mo,W metal; X=S,Se chalcogen) are semiconductors formed by quasi-2D X-M-X layers stacked by weak Van-der-Waals forces. They exhibit an indirect-bandgap in the near-infrared spectral range and band-edges located between the maximum of the valence band at the  $\Gamma$  point and the minimum of the conduction band at the Q point. The direct bandgap is in the visible spectrum, with the band-edges located at energy-degenerate valleys ( $K\pm$ ) at the corners of the Brillouin zone.

Here we identify indirect-bandgap excitons in large-area monolayer WSe<sub>2</sub> both in the absorption spectrum and in the emission with  $\mu$ s-long lifetime. We provide direct experimental evidence that direct and indirect excitons coexist and give rise to distinct emission peaks. Near absolute zero temperature, the indirect excitonic emission peak is almost two orders of magnitude higher than the direct one, thus proving that monolayer WSe<sub>2</sub> is an indirect-bandgap semiconductor. At room temperature, fast non-radiative channels outpace the emission from indirect-bandgap excitons, and only direct-bandgap transitions are detectable. We conclude that it is not correct to infer the bandgap nature from the emission spectra at room temperature without time decays. The richness of excitonic states in WSe<sub>2</sub>, featuring fast and slow-lived states as well as spin dependence, will enable novel photon-exciton interaction schemes with possible applications in quantum information processing, telecommunication and energy.



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