Theory of incommensurate multi-shell nanowires

Young-Woo Son
Korea Institutie for Advanced Study

Cylindrical multishell structure is one of prevalent atomic arrangements in nanowires. Being multishell, the well-defined atomic periodicity is hardly realizable in it because the periodic units of individual shells therein cannot match well except very few cases, posing a challenge to understand its physical properties. Here we show that moire patterns generated by superimposing atomic lattices of individual shells are decisive in determining its electronic structures. Double-walled carbon nanotubes, as an example, are shown to have spectacular variations in electronic properties from metallic to semiconducting and further to insulating states depending on their moire patterns even though they have only semiconducting nanotubes with almost similar energy gaps and diameters. Thus, aperiodic multishell nanowires can be classified into new one-dimensional moire crystals with distinct electronic structures.