Joint CQSE and CASTS Seminar

Weekly Seminar
Apr. 26, 2013 (Friday)

TIME Apr. 26, 14:30 ~ 15:30

TITLE Graphene, Graphane, and Topological Surface States of Bi Thin Films

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<u>Abstract</u>

The electronic structure of graphane with hydrogen vacancies, which are supposed to occur in the process of hydrogenation of graphene, is investigated. A variety of configurations is considered and defect states are derived by density functional calculation. We find that a continuous chain-like distribution of hydrogen vacancies will result in conduction of linear dispersion. The same conduction also occurs for chain-like vacancies in an otherwise fully fluorine-adsorbed graphene. We also find that the structure consisting of an armchair single-walled carbon nanotube deposited on a graphene nanoribbon is greatly strengthened by the further adsorption of titanium or vanadium chain. DFT calculations show that the nanotube and nanoribbon are firmly ”glued” together by the atomic chain introduced between them. Band structures reveal strong hybridization between the 3*d* orbitals of the transition metals and 2*p* orbitals of the carbon atoms. For Ti adsorption at the ribbon center, the chain is nonmagnetic while the ribbon remains antiferromagnetic. For adsorption at the edge, however, magnetism totally disappears at the coupling side. Magnetism for V chain adsorption is even more complicated. The results point to a new way for synthesizing nanowires and possible application in robust nanoelectronic circuits.

We also use density functional calculations to investigate the electronic structure of the four-bilayer Sb film and find that adsorptions of nonmagnetic impurity atoms of hydrogen and 3*d* transition-metal atoms on the film all close the energy gap of the free-standing film and facilitate the formation of Dirac cones that preserve time-reversal symmetry. However, magnetic atoms of the 3*d* transition metals do just the opposite. The results suggest the counterintuitive concept of achieving topological conduction by doping nonmagnetic impurity atoms on thin films of topological insulators.