Intriguing Properties of Inorganic Nanographenes: From Boron Nitride to Silicon Carbide and Molybdenum Disulfide

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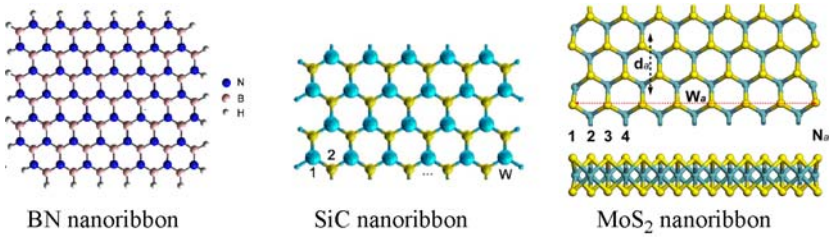
The carbon nanographene ribbons have a unique electronic structure critically depending on the edge shapes, and these properties endow graphene-based materials many applications. Such planar structures are not limited to carbon, the inorganic nanoribbons also exhibit many intriguing properties. In this talk, we will present our recent efforts in exploring the intrinsic properties of inorganic nanoribbons by means of density functional computations.

Boron nitride nanoribbons: In contrast to carbon graphenes, the HOMO-LUMO energy gaps of BN nanographenes (BNNGs) have a weak dependence with size, all BNNGs have closed-shell singlet ground states, and those with long zigzag edges have only slightly lower gap energies.[1]

Silicon carbide nanoribbons: The isoelectronic zigzag SiC nanoribbons are magnetic metal, whose spin polarization originates from the unpaired electrons localized on the ribbon edges. Interestingly, the zigzag SiC nanoribbons narrower than ~4 nm present half-metallic behavior. Without the aid of external field or chemical modification, the metal-free half-metallicity predicted for narrow SiC zigzag nanoribbons opens a facile way for nanomaterial spintronics applications. [2]

MoS_2 nanoribbons: Zigzag nanoribbons show the ferromagnetic and metallic behavior, while armchair nanoribbons are nonmagnetic and semiconducting. The higher stability of MoS_2 nanoribbons, compared with the experimentally available triangular MoS_2 nanoclusters, invites the experimental realizations of such novel ribbons in true nanoscale.[3]



BN nanoribbon SiC nanoribbon MoS_2 nanoribbon

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