DFT calculation of rectangular MoS_2 nanotubes

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Introduction: Two-dimensional atomic layered materials represented by graphene have attracted extensive attention from researchers, because of their rich variety of physical and chemical properties. These materials also show broad application prospects in the electronic devices, optoelectronic devices, catalysts and energy fields. MoS_2 is one of the representatives of these materials. In the previous study, we have successfully synthesized MoS_2 nanotubes using thermal CVD with FeO nanoparticle catalysts [1]. The cross section of the MoS_2 nanotubes showed rectangular shape, which is different from cylindrical ones typically observed in carbon nanotubes. In order to examine the origin of this unusual shape, here we report DFT calculations to see the stability and electronic structures of rectangular MoS_2 nanotubes.

Computational details: We used Vienna Ab-initio Simulation Package (VASP) with Projector Augmented Wave (PAW) potential. Plane waves with kinetic energy cutoff of 500eV. The generalized gradient approximation of Perdew-Buker–Ernzerhof (GGA-PBE) is adopted for exchange-correlation functional. Brillouin zone sampling was performed with Monkhorst-Pack special-points meshes of 1×1×7 k-points. A vacuum layer larger than 15Å was added to avoid the interaction between the neighboring tubes. The lattice constants and all atomic positions were fully relaxed until the atomic forces were smaller than 0.03 eV.

Results: After optimization of the structure, the cell parameters of the nanotubes are $\alpha = \beta = \gamma = 90°$, demonstrating at least metastability of these rectangular structures. Some structures are shown in Fig. 1. The free energies of rectangular nanotubes are less than that of cylindrical ones with the same size when the Mo atom number in the roll is less than 24~32 (i.e. [8,8]), but they are greater when the number is greater. The bandgaps of the rectangular nanotubes were much less than cylindrical ones. Armchair type rectangular nanotube has only 0.2~0.3eV bandgap. HOMO and LUMO are shown in Fig. 2. We consider the sharp edges of the structure strongly affect the electronic structure of nanotubes.

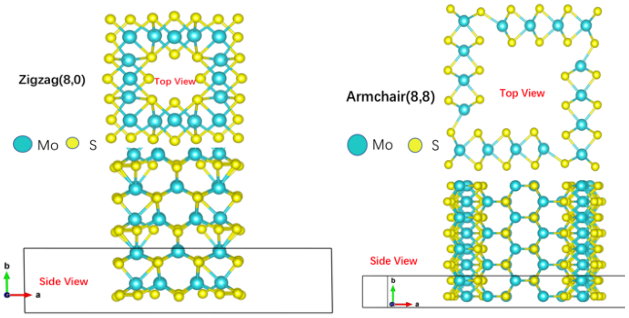

Fig.1. Optimized MoS_2 nanotube structures.

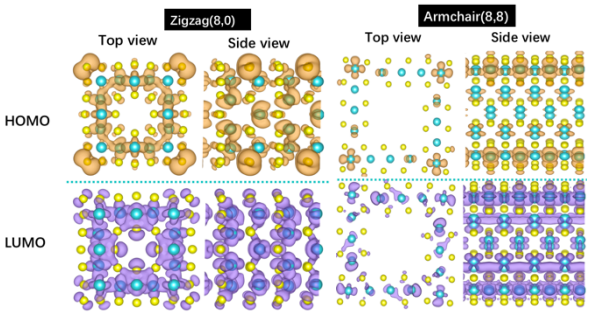

Fig. 2. HOMO-LUMO.

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