Energetics and electronic properties of Janus WSSe

Yanlin Gao, Susumu Okada
University of Tsukuba
E-mail: ylgao@comas.tsukuba.jp

Janus transition metal dichalcogenides (TMDC) have a structural asymmetry with respect to their atomic layer, since its transition metal layer is sandwiched by different chalcogen layers. Experiments reported unique structural and physical properties such as intrinsic scrolling, Rashba spin splitting, piezoelectric polarization, and second-harmonic generation, owing to the structural symmetry. Therefore, the Janus TMDCs have been attracting much attention in pure and applied sciences. Although many theoretic works elucidated fundamental properties of Janus TMDCs, the comprehensive knowledge about the energetics and electronic structures of Janus TMDCs are not yet addressed. Therefore, in this work, we studied the energetics and electronic structures of Janus WSSe to elucidate its structural properties by considering the armchair nanotubes with the density functional theory.

Our results showed that the total energy per atom of WSSe nanotube relative to that of an isolated monolayer WSSe decreases with increasing its diameter. Interestingly, the total energy of the tubular structure with the diameter of 46 Å or larger is lower than that of the isolated WSSe sheet. Thus, Janus WSSe intrinsically possesses the scrolled or tubular structure as its ground state without the supporting substrates. With further increase of the diameter, the total energy saturated 8 meV/atom at the diameter of 67 Å or larger. The WSSe nanotubes are semiconductors whose low-energy band spectra are sensitive to their diameter and Se arrangement in the tubular structure. The tube with large diameter has the similar band edge arrangement to that of the isolated WSSe sheet. While the tubes with small diameter or Se inside arrangement have shallow valence band edge energy at the Γ point owing to the strain and dipole effects.

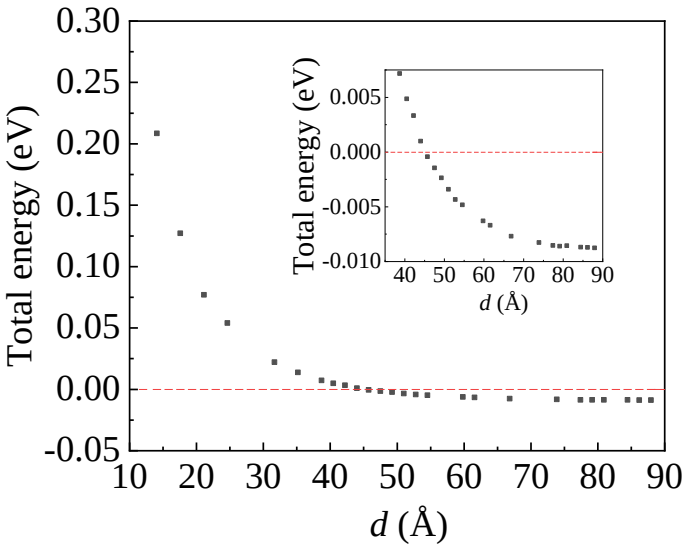

Fig. 1 The total energy per atom of WSSe nanotube, where Se atoms are arranged in outer-most wall as a function of diameter of tube. The energy is measured from that of an isolated monolayer WSSe. An inset is the enlarged around the diameter of 46 Å.