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論文要約

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論文題目 Thesis Title	Geometries and Electronic Properties of Transition Metal Dichalcogenide 2D Layers and Nanotubes: A First-Principles Study

We study geometries and electronic properties of transition metal dichalcogenide (TMD) 2D layers and nanotubes by using the local density approximation in the framework of the density-functional theory.

First, we report the geometric and electronic properties of zigzag MoXY (X, Y = O, S, and Se) nanotubes. We explain that the geometries of zigzag TMD nanotubes can be fully expressed using six independent geometrical parameters, and we give the optimized parameter values for series of MoXY nanotubes. We show that the MoXY nanotubes with smaller chalcogen elements inside (MoSSe, MoOS, and MoOSe) have a preferable natural radius. We further reveal the geometric and electronic properties of these MoXY nanotubes under the uniaxial strains up to ±15%. We find that the mixed-chalcogen TMD nanotubes have larger fundamental gap values compared to TMD nanotubes with single chalcogen species regardless of the value of the strain. The gap properties of all studied oxygen-included TMD nanotubes (MoO_2, MoOS, and MoOSe) exhibit higher strain sensitivity in broad strain region, which will be prospective for applications for mechanical devices such as strain sensors.

Next, we focus on the geometries and the electronic properties of planar MoXY under biaxial and uniaxial strains. We compare these results with MoXY nanotubes. By carefully examining the relationships between the actual geometries and the gap values, we find a global strong correlation between fundamental gap values and some combined geometrical parameters. Because all MoXY (X, Y = S, and Se) nanotubes studied and all planar MoXY (X, Y =, S, and Se) studied are confirmed to align in this single relationship regardless of strains, we consider that this relationship will enable one to predict the gap values of MoXY layered materials with much less computational resources.

We report some new MoS_2 nanostructures obtained in the study of MoS_2 nanotubes. We find that our structures achieve the lowest total energy in a specific condition. We analyze the detailed geometry, and construct generalized geometries. We analyze the energetical stability of these generalized MoS_2 structures by assuming a simple energetic model. We also present the band structures of the new MoS_2 structures.