Title: Evolution of structural and electronic properties standardized description in rhenium disulfide at the bulk-monolayer transition

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Abstract: The structural and electronic properties of ReS2 different forms — three-dimensional bulk and two-dimensional monolayer — were studied within density functional theory and pseudopotentials. A method for standardizing the description of bulk unit cells and "artificial" slab unit cells for DFT research has been proposed. The preference of this method for studying zone dispersion has been shown. The influence of the vacuum layer thickness on specified special high-symmetry points is discussed. Electron band dispersion in both classical 3D Brillouin zones and transition to 2D Brillouin zones in the proposed two-dimensional approach using the Niggli form of the unit cell was compared. The proposed two-dimensional approach is preferable for low-symmetry layered crystals such as ReS2. It was established that the bulk ReS2 is a direct gap semiconductor (band gap of 1.20 eV), with the direct transition lying in the X point of the first Brillouin zone, and it is in good agreement with published experimental data. The reduction in material dimension from bulk to monolayer was conducted with an increasing band gap up to 1.45 eV, with a moving direct transition towards the Brillouin zone center. The monolayer of ReS2 is a direct-gap semiconductor in a wide range of temperatures, excluding only a narrow range at low temperatures, where it comes as a quasi-direct gap semiconductor. The transition, situated directly in the Γ-point, lies 3.3 meV below the first direct transition located near this point. The electronic density of states of ReS2 in the bulk and monolayer cases of ReS2 were analyzed. The molecular orbitals were built for both types of ReS2 structures as well as the electron difference density maps. For all types of ReS2 structures, an analysis of populations according to Mulliken and Voronoi was carried out. All calculated data is discussed in the context of weak quantum confinement in the 2D case.

Keywords: Rhenium disulfide, Slab, Monolayer, Density functional theory, Pseudopotential theory, Electronic structure, Density of states, Molecular orbitals, Electronic density

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