Abstract Submitted
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A *first principles* investigation of point defects in monolayer, few-layer, and bulk WS_2[1] WUN-FAN LI, CHANGMING FANG, MARJOLEIN DIJKSTRA, MARIJN A. VAN HUIS, Soft Condensed Matter, Debye Institute for Nanomaterials Science, Utrecht University, SOFT CONDENSED MATTER TEAM — We present the results of a systematic study of physics of point defects in 2D WS_2 materials conducted by means of density functional theory. First, we investigate the physics of point defects in monolayer (ML) WS_2. Second, we examine the impact of point defects on the physical properties of multi-layer defective WS_2 as a function of slab thickness. The studied point defects are: monovacancies, interstitials and anti-sites, and the considered physical properties include local geometry, defect formation energy, electronic structure and magnetism. Van der Waals interaction, spin-polarization and spin-orbit coupling effects are also incorporated in the calculations to ensure accurate results. In a ML WS_2, we predict that I_S is the most favorable defect inside WS_2 having a low formation energy of 1.21 eV. W_S and W_{S2} anti-sites result in a total magnetic moment of 2 μ_B. By studying ML, few-layer (up to 4 layers), and bulk WS_2 slabs we find that, all point defects cause only localized perturbation, thus have little influence on the thickness-dependent evolution of the physical properties. The depth-dependence of the defect formation energy is also found: V_S prefers to stay on the surface, while V_W prefers the slab center.

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