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Structural and electronic properties of transition metal chalcogenides (MoS₂, Mo₂S₄, and Mo₆S₈)

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Abstract :

Layered transition metal chalcogenides are inorganic materials similar to the graphene, but in contrast to graphene some of the transition metal chalcogenides, such as molybdenum disulfide (MoS₂), have an intrinsic band gap. A band gap is a property essential for many applications including low dimensional transistors, optoelectronic devices and solar energy harvesters. MoS₂ has a layered structure with each layer consisting of S-Mo-S sheets, consisting of an atomic plane of Mo sandwiched between two atomic planes of S in trigonal prismatic arrangement. While atoms in each layer are strongly bound, layers are attracted to each other by weak van der Waals forces conferring on MoS₂ an anisotropic structure, and anisotropic electrical, optical, and mechanical properties [1,2,3]. We present the structural and elastic properties of three materials (MoS₂, Mo₂S₄, and Mo₆S₈) predicted using Density functional theory (DFT) with the inclusion of Van der Waals interactions. The obtained equilibrium structural parameters for these materials agree with experimental data. The calculated cohesive energy and formation energy show that these materials are stable. Apart from above properties we present also the electronic properties (band gaps) of these three materials by the many-body perturbation theory in the GW approximation, currently the most accurate first-principles approach for electronic band structure of extended systems. The obtained band gaps agree with the experimental data. [1] A. Kumar and P. Ahluwalia, Electronic structure of transition metal dichalcogenides monolayers 1 H-MX₂ (M=Mo, W; x= S, Se, Te) from ab-initio theory: new direct band gap semiconductors, The European Physical Journal B-Condensed Matter and Complex Systems, vol. 84, no. 6, pp. 1 – 7, 2012. [2] O. Sedelnikova, L. Bulusheva, and A. Okotrub, Ab initio study of dielectric response of rippled graphene, The Journal of chemical physics, vol. 134, no. 24, pp. 244707 – 244707, 2011. [3] D. Late, B. Liu, H. Matte, C. Rao, and V. Dravid, Rapid characterization of ultrathin layers of chalcogenides on SiO₂/Si substrates, Advanced Functional Materials, 2012.

Award :

No

Paper :

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