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Structural and electronic properties of transition metal chalcogenides (MoS2 , Mo2 S4 , and Mo6 S8)

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Abstract content
   (Max 300 words)

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 transitors, 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.

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[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.

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