

Abstract Submitted
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Electronic and optical properties of single-layer, double-layer, and bulk SnSe and GeSe EMMANOUIL KIOUPAKIS, GUANGSHA SHI, Materials Science and Engineering, University of Michigan — We used density functional and many-body perturbation theory to calculate the quasiparticle band structures and optical properties of single-layer, double-layer, and bulk SnSe and GeSe. The calculated direct and indirect band gaps of the bulk materials are in good agreement with experiment. While the electronic band gaps increase by up to 600 meV in the single-layer, double-layer, and bulk SnSe, the transition energy of the $n = 1$ exciton does not change as a function of thickness. The same trend was also discovered in GeSe. The fundamental band gaps were found to be direct in SnSe and GeSe monolayers. We calculated the absorption spectra for both the bulk and 2-dimensional systems, and determined the light absorbance for light polarization along the in-plane arm-chair and zigzag directions. This research was supported by the National Science Foundation CAREER award through Grant No. DMR-1254314. Computational resources were provided by the DOE NERSC facility.

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