

Abstract Submitted
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Electronic structure and lattice dynamics of few-layer InSe¹ LUCAS WEBSTER, JIA-AN YAN, Department of Physics, Astronomy and Geosciences, Towson University — Studies of Group-III monochalcogenides (MX, M = Ga and In, X = S, Se, and Te) have revealed their great potentials in many optoelectronic applications, including solar energy conversion, fabrication of memory devices and solid-state batteries. Among these semiconductors, indium selenide (InSe) has attracted particular attention due to its narrower direct bandgap, which makes it suitable for photovoltaic conversion. In this work, using first-principles calculations, we present a detailed study of the energetics, atomic structures, electronic structures, and lattice dynamics of InSe layers down to two-dimensional limit, namely, monolayer InSe and bilayer InSe with various stacking geometry. Calculations using various exchange-correlation functionals and pseudopotentials are tested and compared with experimental data. The dependence of the Raman spectra on the stacking geometry and the laser polarization will also be discussed.

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