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Band gap engineering of Zn based II-VI semiconductors through uniaxial strain SATYESH YADAV, RAMPI RAMPRASAD, University of Connecticut — The electronic structure of bulk wurtzitic ZnX (X=O, S, Se, and Te) under uniaxial strain along the [0001] direction is investigated using hybrid density functional theory calculations and many-body perturbation theory. It is found that uniaxial tensile and large compressive strains decrease the band gap, similar to what has been predicted by semilocal density functional theory (DFT) calculations [Yadav et. al, Phys. Rev. B, **81**, 144120 (2010)]. Moreover, the change in the band gap under uniaxial strains predicted by semilocal DFT is in good quantitative agreement with the present results at all strains considered, thereby bringing a measure of redemption to conventional (semi)local DFT descriptions of the electronic structure of at least this class of insulators. The present results have important implications for band gap engineering through strain, especially for complex systems containing a large number of atoms (e.g., nanowires) for which higher-level calculations may be too computationally intensive.

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