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ZnX (X = O, S, Se, Te) under uniaxial strain[1] SATYESH YADAV, THOMAS SADOWSKI, R. RAMPRASAD, University of Connecticut — We present a first principles density functional theory based study of the impact of uniaxial strain on the structural and electronic properties of bulk ZnX (X = O, S, Se, Te) in the wurtzite and zinc blende phases. The strain axis was chosen to be along the [0001] and [111] directions, respectively, for the wurtzite and zinc blende systems. For large uniaxial compressive strains, all systems undergo a transition from the equilibrium wurtzite or zinc blende phases (which display sp^3 hybridization) to a graphite-like phase (displaying sp^2 hybridization). Simultaneously, the band gap of the systems gradually drops to a small or zero value. Under large uniaxial tensile strains, all systems tend to form individual stoichiometric ZnX layers, also with small band gap values relative to the corresponding equilibrium ones. Although the range of strains considered here is enormous, appreciable changes (i.e, reductions) of the band gap may be accomplished for modest and realistic strains achievable in nanowires.

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