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Structural and electronic properties of high pressure phases of lead chalcogenides JOHN PETERSEN, LUISA SCOLFARO, THOMAS MYERS, Texas State University — Lead chalcogenides, most notably PbTe and PbSe, have become an active area of research due to their thermoelectric properties. The high figure of merit (ZT) of these materials has brought much attention to them, due to their ability to convert waste heat into electricity. Variation in synthesis conditions gives rise to a need for analysis of structural and thermoelectric properties of these materials at different pressures. In addition to the NaCl structure at ambient conditions, lead chalcogenides have a dynamic orthorhombic (Pnma) intermediate phase and a higher pressure yet stable CsCl phase. By altering the lattice constant, we simulate the application of external pressure; this has notable effects on ground state total energy, band gap, and structural phase. Using the General Gradient Approximation (GGA) in Density Functional Theory (DFT), we calculate the phase transition pressures by finding the differences in enthalpy from total energy calculations. For each phase, elastic constants, bulk modulus, shear modulus, Young's modulus, and hardness are calculated, using two different approaches. In addition to structural properties, we analyze the band structure and density of states at varying pressures, paying special note to thermoelectric implications.

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