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Pressure induced structural transitions in Lead Chalcogenides and its influence on thermoelectric properties JOHN PETERSEN, MICHAEL SPINKS, Department of Physics, Texas State University, San Marcos, Texas, PABLO BORGES, Instituto de Ciências Exatas e Tec., Universidade Federal de Viçosa, Rio Paranaiba, MG, Brazil, LUISA SCOLFARO, Department of Physics, Texas State University, San Marcos, Texas — Lead chalcogenides, most notably PbTe and PbSe, have become an active area of research due to their thermoelectric (TE) 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, with a possible application being in engine exhaust. Here, we examine the effects of altering the lattice parameter on total ground state energy and the band gap using first principles calculations performed within Density Functional Theory and the Projector Augmented Wave approach and the Vienna Ab-initio Simulation Package (VASP-PAW) code. Both PbTe and PbSe, in NaCl, orthorhombic, and CsCl structures are considered. It is found that altering the lattice parameter, which is analogous to applying external pressure on the material experimentally, has notable effects on both ground state energy and the band gap. The implications of this behavior in the TE properties of these materials are analyzed.

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