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Theoretical study of the structural, vibrational and dielectric properties of PbSnTe alloys HORACIO W. LEITE ALVES, ANTONIO R.R. NETO, Univ. Fed. de Sao Joao del Rei, JOHN E. PETERSEN, Texas State University, PABLO D. BORGES, Univ. Fed. de Viçosa, LUISA M.R. SCOLFARO, Texas State University — Thermoelectric devices have promise in dealing with the challenges of the growing demand for alternative clean energy and Te-based materials well-known candidates for them. Recently [1], we have shown that the high values for the dielectric constant, together with anharmonic LA-TO coupling, reduces the lattice thermal conductivity and enhances the electronic conductivity in PbTe. Also, it was shown that by alloying this material with Se, the electronic conductivity of the alloys is also enhanced [2]. But, it is not clear if the same occurs when alloying with Sn. We show, in this work, our *ab initio* results for the structural, vibrational and dielectric properties of $Pb_{1-x}Sn_xTe$ alloys. The calculations were carried out by using the Density Functional Theory, and the alloys were described by the Virtual Crystal Approximation. Our results show that their structural properties do not obey the Vegard rule. However, we have detected that the anharmonic LA-TO coupling still exists and the obtained values for the dielectric constant show higher values than that obtained for PbTe.

[1] H. W. Leite Alves, *et al.*, Phys. Rev. B87, 115204 (2013).
[2] Y. Pei, *et al.*, Nature 473, 66 (2011).

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