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Anomalous Temperature dependent band gap in Black Phosphorus ALEXANDRE REILY ROCHA, CESAR PEREZ VILLEGAS, Institute for Theoretical Physics, State University of Sao Paulo, Brazil, ANDREA MARINI, Istituto di Struttura della Materia of the National Research Council and European Theoretical Spectroscopy Facility, Italy — Black phosphorus has a number of electronic and optical properties, which are associated with it anisotropic structure. In terms of thermal properties, one poorly understood phenomena is black phosphorus' band gap temperature dependence. It presents a behaviour, which is opposite to most semiconductors, when temperature is increased, the fundamental band gap increases instead of decreases. In this work, based on ab initio density functional perturbation theory calculations, we present an explanation for this long known and yet not fully explained effect. We show that it arises from a combination of harmonic and lattice thermal expansion contributions. We narrow down the origin of this this effect to specific vibrational modes that present anharmonic contributions [1]. [1] C. P. Villegas, A. R. Rocha, A. Marini, Nano Lett., 16, 5095 (2016).

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