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Ab-Initio Computations of Electronic and Related Properties of cubic Lithium Selenide (Li_2Se) ABDOULAYE GOITA, Department of Electrical Engineering, Southern University and AM College, Baton Rouge, IFEANYI H. NWIGBOJI, Department of Computational Science, University of Texas at El Paso, El-Paso, TX 79968 USA, YURIY MALOZOVSKY, DIOLA BAGAYOKO, Department of Physics, Southern University and AM College, Baton Rouge, LA 70813, USA
— We present theoretical predictions, from ab-initio, self-consistent calculations, of electronic and related properties of cubic lithium selenide (Li_2Se). We employed a local density approximation (LDA) potential and the linear combination of atomic orbitals (LCAO). We performed the computations following the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF). Our results include electronic energies, total and partial densities of states, effective masses, and the bulk modulus. The theoretical equilibrium lattice constant is 5.882 Å. We found cubic Li_2Se to have a direct band gap of 4.363 eV (prediction), at Γ. This gap is 4.065 eV for a room temperature lattice constant of 6.017 Å. The calculated bulk modulus is 31.377 GPa. Acknowledgments: This work was funded in part by the National Science Foundation (NSF) and the Louisiana Board of Regents, through LASiGMA [Award Nos. EPS- 1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, the US Department of Energy – National, Nuclear Security Administration (NNSA) (Award No. DE- NA0002630), LaSPACE, and LONI-SUBR.

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