

Abstract Submitted
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Ab-initio Calculation of Optoelectronic and Structural Properties of Cubic Lithium Oxide (Li_2O). JOSHUA ZIEGLER, Department of Physics, Case Western Reserve University, Cleveland, OH 44106, USA, DANIEL POLIN, Department of Physics, New York University, New York City, NY 10003, USA, YURIY MALOZOVSKY, DIOLA BAGAYOKO, Department of Physics, Southern University and AM College, Baton Rouge, LA 70813, USA — Using the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF), we performed ab-initio, density functional theory (DFT) calculations of optoelectronic, transport, and bulk properties of Li_2S . In so doing, we avoid “band gap” and problems plaguing many DET calculations [AIP Advances 4, 127104 (2014)]. We employed a local density approximation (LDA) potential and the linear combination of atomic orbitals (LCAO). With the BZW-EF method, our results possess the full, physical content of DFT and agree with available, corresponding experimental ones. In particular, we found a room temperature indirect band gap of 6.659 eV that compares favorably with experimental values ranging from 5 to 7.99 eV. We also calculated total and partial density of states (DOS and PDOS), effective masses of charge carriers, the equilibrium lattice constant, and the bulk modulus. 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 Nos. DE-NA0001861 and DE- NA0002630), LaSPACE, and LONI-SUBR.

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