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Ab-initio Density Functional Theory (DFT) Studies of Electronic, Transport, and Bulk Properties of Sodium Oxide (Na_2O). DANIEL POLIN, Department of Physics New York University, New York, NY 10003, USA, JOSHUA ZIEGLER, Department of Physics Case Western Reserve University, Cleveland, OH 44106, USA., YURIY MALOZOVSKY, DIOLA BAGAYOKO, Department of Physics Southern University and AM College, Baton Rouge, LA 70813, USA. — We present the findings of *ab-initio* calculations of electronic, transport, and structural properties of cubic sodium oxide (Na_2O). These results were obtained using density functional theory (DFT), specifically a local density approximation (LDA) potential, and the linear combination of Gaussian orbitals (LCGO). Our implementation of LCGO followed the Bagayoko, Zhao, and Williams method as enhanced by the work of Ekuma and Franklin (BZW-EF). We describe the electronic band structure of Na_2O with a direct band gap of 2.22 eV. Our results include predicted values for the electronic band structure and associated energy eigenvalues, the total and partial density of states (DOS and pDOS), the equilibrium lattice constant of Na_2O, and the bulk modulus. We have also calculated the electron and holes effective masses in the Γ to L, Γ to X, and Γ to K directions. 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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