Abstract Submitted
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Accurate Electronic, Transport, and Structural Properties of Disodium Sulfide (Na_2S) WALTER LYNN, Carleton College, Northfield, MN, BETHUEL KHAMALA, YURIY MALOZOVSKY, DIOLA BAGAYOKO, Southern Univ & A&M College — We present results of *ab-initio*, self consistent calculations of electronic, transport, and structural properties of cubic antifluorite disodium sulfide (Na_2S). We used a local density approximation (LDA) potential and the linear combination of Gaussian orbitals (LCGO) formalism. We followed the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF), in our implementation of the LCGO. We discuss electronic energy bands, total (DOS) and partial (pDOS) densities of states, effective masses that are pertinent to transport properties, and the bulk modulus. For a room temperature lattice constant of 6.539 Å, our calculated, direct band gap of the material, at Γ, is 2.83 eV. We predict a direct band gap of 3.05 eV for the calculated equilibrium lattice constant of 6.395 Å. The significant decrease of the lattice constant, for a drop in temperature from 300 to 0 K, is understandable with the relatively small, predicted bulk modulus of 43.9 GPa. Acknowledgments: This work was funded in part by the 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 – NNSA (Award Nos. DE-NA0001861 and DE- NA0002630), LaSPACE, and LONI-SUBR.

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