Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

DFT Predictions of Electronic, Transport, and Bulk Properties of Li_2S YURIY MALOZOVSKY, LASHOUNDA FRANKLIN, Southern Univ & A&M Coll, CHINEDU EKUMA, Louisiana State University and A&M College, DIOLA BAGAYOKO, Southern Univ & A&M Coll — We present results from *ab-initio,* self consistent calculations of electronic, transport, and bulk properties of cubic antifluorite (anti-CaF_2) lithium sulfide (Li_2S). Our computations employed the local density approximation (LDA) potential of Ceperley and Alder and the linear combination of atomic orbital (LCAO) formalism. The implementation of the LCAO formalism followed the Bagayoko, Zhao, and Williams method, as enhanced by Ekuma and Franklin (BZW-EF). Consequently, we solved self consistently both the Kohn-Sham equation and the one giving the ground state charge density in terms of the wave functions of the occupied states. For a low temperature lattice constant, our calculated, indirect gap, from Γ to X, is 3.723. The predicted LDA band gap is 3.702 eV. We discuss the total and partial densities of states, electron and hole effective masses, and the predicted bulk modulus of 45.57 GPa that agrees with a low temperature measurement of 45.7 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 Nos. DE-NA0001861 and DE-NA0002630), LaSPACE, and LONI-SUBR.

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Date submitted: 12 Nov 2014 Electronic form version 1.4