Abstract Submitted for the MAR14 Meeting of The American Physical Society

Ab-initio Calculations of Accurate Electronic Properties of ZnS BETHUEL KHAMALA, LOUSHANDA FRANKLIN, YURIY MALOZOVSKI, ANTHONY STEWART, DIOLA BAGAYOKO, Southern Univ & A&M Coll, BAGAYOKO RESEARCH GROUP TEAM — We present the results from ab*initio*, self consistent, local density approximation (LDA) calculations of the electronic and related properties of zinc-blende zinc sulphide (zb-ZnS). We employed the Ceperley and Alder LDA potential and the linear combination of atomic orbital (LCAO) formalism in our non-relativistic computations. The implementation of the LCAO formalism followed the Bagayoko, Zhao, and Williams method as enhanced by Ekuma and Franklin (BZW-EF). The BZW-EF method includes a methodical search for the optimal basis set that yields the minima of the occupied energies. This search entails increasing the size of the basis set and related modifications of angular symmetry and of radial orbitals. Our calculated, direct gap of 3.725 eV, at the Γ point, is in excellent agreement with experiment. We have also calculated the total (DOS) and partial (pDOS) densities of states, electron and hole effective masses and total energies that agree very well with available, corresponding experimental results. Acknowledgement: This research is 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-NA0001861), LaSPACE, and LONI-SUBR.

> Bethuel Khamala Southern Univ & A&M Coll

Date submitted: 15 Nov 2013

Electronic form version 1.4