Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

***Ab-initio* Calculations of Accurate Electronic Properties of Wurzite AlN** IFEANYI NWIGBOJI, YURIY MALOZOVSKY, DIOLA BAGAYOKO, Southern Univ & A&M Coll, BAGAYOKO RESEARCH GROUP TEAM — We present results from *ab-initio*, self consistent local density approximation (LDA) calculations of electronic and related properties of wurtzite Aluminum Nitride (w-AlN). Our non-relativistic computations employed the Ceperley and Alder LDA potential 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). The BZW-EF method verifiably obtains the minima of the occupied energies; these minima provide the most variationally and physically valid density functional theory (DFT) description of the ground states of materials under study. Our preliminary results for w-AlN show that w-AlN has a direct band gap of 5.82 eV at the Γ point. The preliminary energy bands were obtained with a basis set comprising 48 functions. None of the several, larger basis sets tested to date led to occupied energies lower than those obtained with the above 48. While most previous LDA calculations are 2 eV smaller or more than the experimental value of 5.9 eV that is in excellent agreement with our finding, considering the typical experimental uncertainty of 0.2 eV for absorption measurements on AlN. We also discuss our calculated density of states (DOS) and partial densities of states (pDOS).

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Date submitted: 15 Nov 2013 Electronic form version 1.4