Abstract Submitted for the MAR06 Meeting of The American Physical Society

Predictions of Electronic and Optical Properties of Cubic InN LASHOUNDA FRANKLIN, HUA JIN, G. L. ZHAO, DIOLA BAGAYOKO, Southern University and A&M College — We present theoretical predictions of electronic, optical, and related properties of cubic indium nitride (c-InN). We utilized a local density functional approximation (LDA) potential and the linear combination of atomic orbitals (LCAO) in our ab-initio, self-consistent calculations that implemented the Bagayoko, Zhao, and Williams (BZW) method. The predicted band gap is 0.65 eV at a theoretical, equilibrium lattice constant of 5.017 Å . We discuss other predictions for the structural and optical properties of c-InN, including the bulk modulus, electron effective masses, and the calculated dielectric function. This work was funded in part by the Department of the Navy, Office of Naval Research (ONR, Grant Nos. N00014-05-1-0009 and N00014-4-1-0587), NASA (Award Nos. NCC 2-1344, NAG 5-10253, and NNG 05G146G), and the National Science Foundation (Award No. HRD 0503362).

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Date submitted: 05 Dec 2005 Electronic form version 1.4