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Calculated, Optical Proprieties of Wurtzite InN DIOLA BAGAYOKO, HUA JIN, GUANGLIN ZHAO, Southern University and A&M College, PHYSICS DEPARTMENT TEAM — We report the results of ab-initio calculations of the dielectric function of wurtzite indium nitride (w-InN). These optical properties are derived from ab-initio energy bands obtained with a local density function approximation (LDA) potential in the Bagayoko, Zhao, and Williams (BZW) implementation of the linear combination of atomic orbital (LCAO) formalism. We practically reproduced the measured, dielectric function (Superlattices and Microstructures 36, 591-597, 2004) at energies up to 6 eV. This agreement is not limited to major peaks; it also includes the fine structures of the shoulders. Indubitably, these findings vindicate density functional theory, in general, and the local density approximation (LDA), in particular, for the correct description of properties of semiconductors – provided the basis-set and variational effect, inherently associated with most calculations, is avoided with the first-principle BZW approach. 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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