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Examination of the Properties of the Ab-Initio Calculations for the Electronic Structure of GaAs and InAs G.L. ZHAO, H. JIN, D. BAGAYOKO, Southern University and A&M College — At present, most of the ab-initio density functional calculations for the studies of the electronic structure of solid state materials utilized non-orthogonal basis sets. The mathematical and physical properties of these methods have not been carefully studied and can be different from those utilizing orthogonal basis sets in quantum mechanics theory. We present some of the mathematical properties of the methods, based on the variational theory of Ritz-process. The utilizations of non-orthogonal basis sets in the ab-initio calculations could lead to a non-uniformity in approaching their solutions. We also studied the properties of the ab-initio calculations for the electronic structure of GaAs and InAs. Acknowledgments: this work was funded in part by NSF (Award No. 0508245) and ONR (Grant No: N00014-05-1-0009).

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