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Ab-initio Electronic, Transport and Related Properties of Zinc Blende Boron Arsenide (zb-BAs) IFEANYI H. NWIGBOJI, Department of Computational Science, University of Texas at El Paso, El-Paso, TX 79968 USA., YURIY MALOZOVSKY, DIOLA BAGAYOKO, Department of Physics, Southern University and AM College, Baton Rouge, LA 70813 — We present results from *ab-initio*, self-consistent density functional theory (DFT) calculations of electronic, transport, and bulk properties of *zinc blende* boron arsenide (zb-BAs). We utilized a local density approximation (LDA) potential and the linear combination of atomic orbital (LCAO) formalism. Our computational technique follows the Bagayoko, Zhao, and Williams method, as enhanced by Ekuma and Franklin. Our results include electronic energy bands, densities of states, and effective masses. We explain the agreement between these findings, including the indirect band gap, and available, corresponding, experimental ones. This work confirms the capability of DFT to describe accurately properties of materials, provided the computations adhere to the conditions of validity of DFT [AIP Advances, 4, 127104 (2014)]. Acknowledgments: This work was 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-NA0002630), LaSPACE, and LONI-SUBR.

Yuriy Malozovsky
Southern Univ
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