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Accurate, Electronic and Transport Properties of Wurtzite Aluminum Nitride (w-AlN) IFEANYI NWIGBOJI, YURIY MALOZOVSKY, LASHOUNDA FRANKLIN, Southern University and A&M College, CHINEDU EKUMA, Louisiana State University, DIOLA BAGAYOKO, Southern University and A&M College — We present results from *ab-initio*, self-consistent calculations of electronic and transport properties of wurtzite aluminum nitride (w-AlN). We utilized a local density approximation (LDA) potential, the linear combination of Gaussian orbitals (LCGO), and the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF). With multiple oxidation states of Al and N, the method led to several sets of calculations with different ionic species as input. LDA requires, for the description of w-AlN, the results of the calculation leading to the lowest, occupied energies. With Al^{3+} and N^{3-} as input, the binding energy was 1.5 eV larger, in magnitude, than those for other ionic inputs; hence, the description of w-AlN is provided by a calculation with these ionic species as input. Our calculated, direct band gap for w-AlN, at the Γ point, is 6.28 eV, in excellent agreement with the 6.28 eV experimental value at 5 K. We discuss the bands, total and partial densities of states, and calculated electron and hole effective masses. Funded in part by the 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 – NNSA (Award No. DE-NA0001861), LaSPACE, and LONI-SUBR.

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