Abstract Submitted
for the TSF21 Meeting of
The American Physical Society

Effects of hydrogen passivation and dipole corrections on density functional theory calculations of supercell-slab models for GaN on diamond interfaces[1] ERIC WELCH, LUISA SCOLFARO, Texas State University — Zinc blende GaN is a heteropolar structure with a non-zero dipole moment that effects the charge density and built-in potential across GaN-semiconductor interfaces. Results are shown here from a hybrid density functional theory study of zinc blende GaN and zinc blende diamond using the supercell slab model; GaN on diamond is a promising interface in high electron mobility transistor applications. Electronic structure calculations show that a type I interface (with a Ga adlayer) between GaN and diamond is stable with an adhesion energy of 0.704 eV/A^2 (4.346 J/m^2). Projecting the density of states onto each supercell layer shows that the diamond charge density intercalates into the first layer of GaN, agreeing with recent experiments. It is shown that pseudo-hydrogen passivation of dangling bonds and dipole corrections, used to account for heteropolar structures of GaN, along with the inclusion of a Ga adlayer work to remove spurious interactions between periodic supercell images and yield energetic results like more complicated structural models e.g., wedge-shaped supercells.

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Date submitted: 12 Aug 2021 Electronic form version 1.4