

Supporting Information

***N*- and *p*-Type Ohmic Contacts at Monolayer Gallium Nitride-Metal Interfaces**

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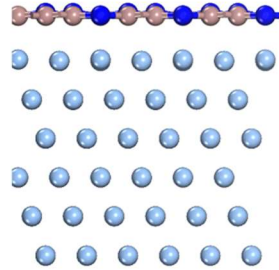
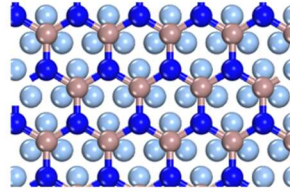
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(a) VASP



(b) ATK

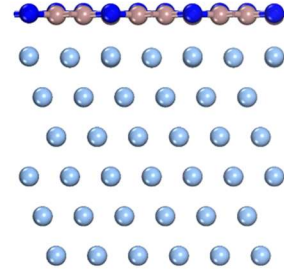
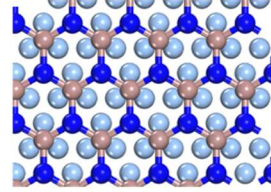
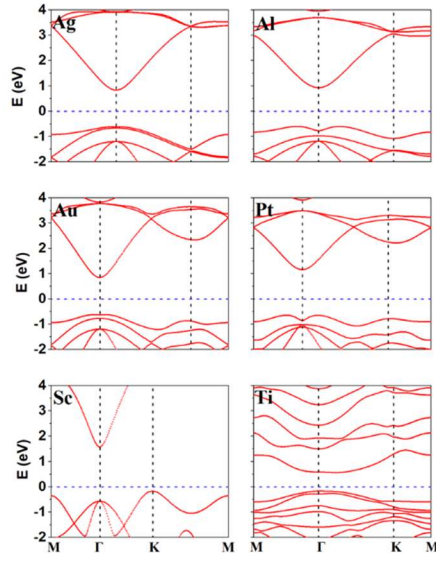


Figure S1. Comparison of the ML planar GaN with Ag electrode optimized by ATK and VASP

(a) planar GaN



(b) buckled GaN

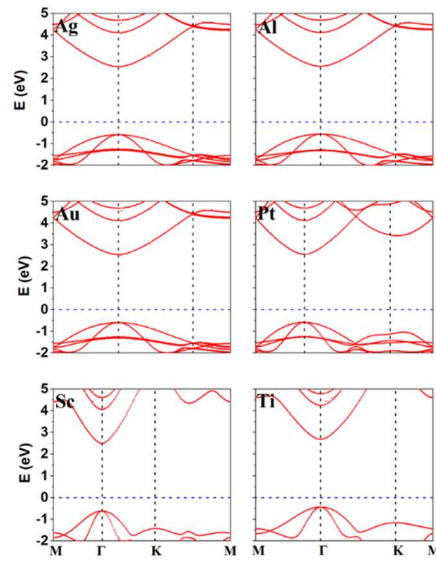


Figure S2. (a) Band structures of ML $\sqrt{3} \times \sqrt{3}$ planar GaN peeled from the stable 2×2 Ag, Al, Au, Pt and Ti electrodes and ML 1×1 planar GaN peeled from the stable 1×1 Sc electrode by the DFT method, respectively. (b) Band structures of ML $\sqrt{3} \times \sqrt{3}$ buckled GaN peeled from the stable 2×2 Ag, Al, Au, and Pt electrodes and ML 1×1 buckled GaN peeled from the stable 1×1 Sc and Ti electrodes by the DFT method, respectively. The Fermi level is at zero energy. Red dots correspond to the states with significant contribution from ML buckled GaN.

buckled GaN/metal

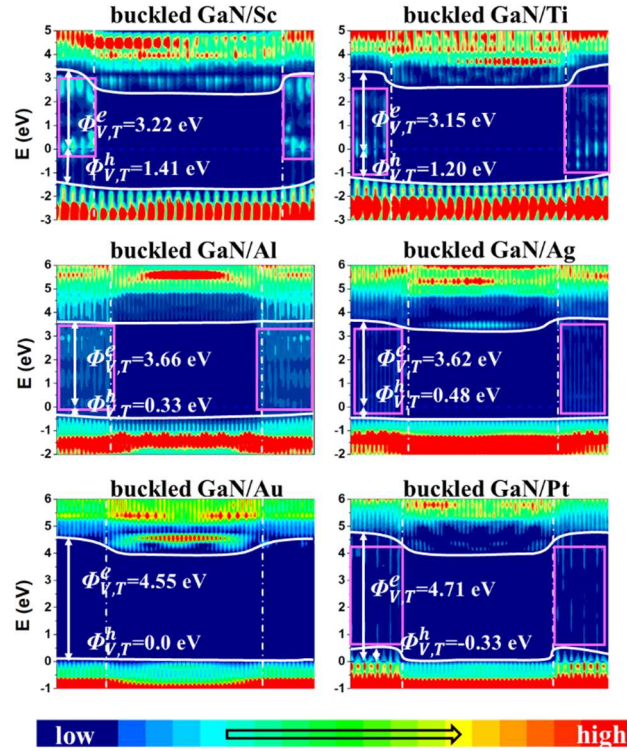


Figure S3. Zero-bias and zero-gate voltage LDOS projected on ML buckled GaN of the ML buckled GaN FET with Sc, Ag, Ti, Al, Au, and Pt electrodes, and the channel length is about 5 nm. Light purple closed area indicates the region with MIGS. The Fermi level is at zero energy. The upright white dashed lines indicate the boundary of ML buckled GaN/metal and the uncontacted ML buckled GaN channel. The responding conduction band and valence band profiles along the channel are given in solid white lines. Light purple closed area indicates the region with MIGS.