Abstract Submitted for the CAL12 Meeting of The American Physical Society

Absolute surface energies of polar and non-polar planes in GaN CYRUS DREYER, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara Materials Department — Growth of high quality single crystals and epitaxial layers of GaN is very important for producing optoelectronic devices. Ab initio calculations can help in determining absolute surface energies, which are key quantities that control crystal-growth rates and fracture toughnesses. By means of hybrid functional calculations, we have determined absolute surface energies for the non-polar  $\{1120\}$  and  $\{1010\}$  and polar (0001) and  $(000\bar{1})$  planes in wurtzite GaN. Low energy reconstructions of the bare and hydrogenated surfaces were considered under various conditions chosen to correspond to growth by molecular beam epitaxy (MBE) or metal-organic chemical vapor deposition (MOCVD). We find that the non-polar planes are close in energy, and lower in energy than the reconstructed  $(000\bar{1})$  polar plane under all conditions considered. The reconstructed (0001) plane is lower in energy than the (0001) plane over the whole range of conditions, and lower in energy than the non-polar reconstructions for Ga-rich chemical potential conditions. From these surface energies, lower bounds on the anisotropic fracture toughness of GaN are determined. Surface energies of polar planes for other III-nitrides will be compared to those of GaN.

> Cyrus Dreyer University of California, Santa Barbara Materials Department

Date submitted: 27 Sep 2012

Electronic form version 1.4