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 \{11\bar{2}0\} and \{1\bar{0}1\} 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 (000\bar{1}) 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