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Atomic and electronic structure of AlN polar surfaces[1]
MAOSHENG MIAO, ANDERSON JANOTTI, CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara — We studied the stability and electronic structure of AlN (0001) and (000-1) polar surfaces using first-principles DFT methods. A plane-wave basis set and PAW potentials are employed surface calculations. In order to correct the band gap of AlN, we applied the hybrid functional in the HSE [1] framework. Using this approach, we obtained a band gap of 6.1 eV, and lattice constants in excellent agreement with experimental values. Under Al-rich conditions, the Al adatom at T4 sites on the Al-terminated (0001) surface was found to be the most stable (2x2) reconstruction. This reconstruction is characterized by occupied surface states (Al-Al bonding) at 3.0 eV below the conduction-band minimum (CBM) and unoccupied surface states (Al dangling bonds) at 1.1 eV below the CBM. Under Al-poor conditions, the N adatom at the H3 site is the most stable reconstruction, with occupied N-Al bonding states at 4.2 eV and an uncoccupied Al dangling-bond state at 1.1 eV below the CBM. For the N-terminated (000-1) polar surface, the structure with an Al adlayer is the most stable under Al-rich conditions. The impact of the surface states on the properties of materials and devices will be discussed. [1] J. Heyd, G.E.Scuseria, and M.Ernzerhof, J. Chem. Phys. 118, 8207(2003).

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