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First principles study of oxidized AlN and GaN nonpolar surfaces[1] MAOSHENG MIAO, CHRIS VAN DE WALLE, Materials Department, Univeristy of California Santa Barbara — We study the reconstructions of oxidized AlN and GaN nonpolar surfaces using first-principles density functional theory. The atomic structures of the surfaces are relaxed using the generalized gradient approximated exchange-correlation functional, and the electronic structures are calculated using the hybrid functional implemented in the Heyd-Scuseria-Ernzerhof (HSE) screened Coulomb potential framework. The stability of surface structures strongly depends on the chemical potentials of Al (Ga) and O. Under cation-rich conditions and in equilibrium with the oxide, the AlN $(10\bar{1}0)$ surface favors a high-density oxide structure formed by O substitution for N (O_N) and O occupation of interstitial sites, while the AlN $(11\bar{2}0)$ surface favors a low-density oxide structure formed by O_N and Al vacancies on the surface. GaN surfaces behave differently, however: under similar conditions, the two GaN non-polar surfaces are oxidized to a structure that consists of only O_N in the top two layers. Despite the substantial change in atomic structure of the surface, the oxidation of nonpolar surfaces does not significantly change the surface states in the gap compared with the bare surfaces, and therefore it does not have significant effect on the electronic properties.

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