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Studies of the atomic structure of the adsorption of B and Al on GaN[1] GREGORIO HERNANDEZ-COCOLETZI, CICESE, CNYN-UNAM, and IF-UAP, Mexico, LUIS PALOMINO-ROJAS, REYES GARCIA-DIAZ, Universidad Autonoma de Puebla, NOBORU TAKEUCHI, Universidad Nacional Autonoma de Mexico — We perform first principles total energy calculations to study the adsorption and diffusion of B and Al on GaN (0001) and (000-1) surfaces, in the (2x2) and ($\sqrt{3}$x$\sqrt{3}$) periodicities. Studies are done within the periodic density functional theory. In the repeated slab geometry method, the slab of the GaN(0001) surface is formed by 4 and 5 bilayers, for the (2x2) and ($\sqrt{3}$x$\sqrt{3}$) periodicities, respectively. The slab of the GaN(000-1) surface is formed by 3 and 4 bilayers, plus a Ga monolayer for the (2x2) and ($\sqrt{3}$x$\sqrt{3}$) periodicities, respectively. Dangling bonds of the bottom surfaces are saturated by pseudo-hydrogen atoms. The two lowest bilayers and the hydrogen are frozen at their ideal positions to simulate the bulk like environment. The upper bilayers and the adsorbed atoms are set free to relax. For the high symmetry sites the most stable structure of the adsorption on the GaN(0001)-(2x2) surface is the T4-site. For the adsorption on the GaN(000-1)-(2x2) is H3.

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