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Interaction of ammonium with a pyridine-like nitrogen-doped graphene (PNG) surface LUIS FERNANDO MAGANA, JUAN M. RAMIREZ, GERARDO JORGE VAZQUEZ, Instituto de Fisica, UNAM — We used density functional theory, with the local density approximation, and molecular dynamics, within the Born-Oppenheimer approximation. We considered the initial position of ammonium just above the PNG vacancy, at 300 K. We performed our calculations using the Quantum Espresso code. The unit cell we considered has one vacancy per twenty-eight carbon atoms, with three nitrogen atoms, and one ammonium molecule. It is found that the PNG vacancy adsorbed strongly one hydrogen atom from the ammonium molecule. Afterwards, the remaining ammonia molecule desorbs.

Luis Fernando Magana
Instituto de Fisica, UNAM

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