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Adsorption of ammonium on a pyridine-like nitrogen-doped graphene layer decorated with a monovalent atom LUIS FERNANDO MAGANA, JUAN M. RAMIREZ, GERARDO JORGE VAZQUEZ, Instituto de Fisica, UNAM — Density functional theory and molecular dynamics were used to study the interaction of an NH_4 molecule with a pyridine-like nitrogen-doped (PNG) surface. The surface is decorated with an impurity taken from the first row of the periodic table. In this way, we considered six different atoms: H, Li, Na, K, Rb and Cs, to decorate the system. We found two final configurations. One, is with the NH_4 molecule physisorbed around the impurity. In the second situation, one hydrogen atom of the ammonium molecule, is adsorbed around a nitrogen atom of the surface. The remaining NH_3 molecule stays physisorbed on the system. The final configuration depends on the initial position of the NH_4 molecule. In all decoration cases, the system was allowed to follow an evolutionary process using molecular dynamics at 300 K, and atmospheric pressure.

Luis Fernando Magana
Instituto de Fisica, UNAM

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