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Ab initio **Studies of Potassium Adsorption on Graphite and Carbon Nanotubes**[1] ALEJANDRO LUGO-SOLIS, IGOR VASILIEV, New Mexico State University — We present an *ab initio* study of a single potassium atom adsorption on the surface of graphite and single walled carbon nanotubes using density functional theory within the pseudopotential approximation. Our study is, in part, inspired by inconsistent results reported for this system in the existing literature. The potassium adsorption energy on graphite obtained in different calculations ranges from approximately 0.4 eV to 1.75 eV. Our calculations demonstrate that the reported disagreements can be explained by electrostatic interactions rather than complex quantum factors. We illustrate this with a simple model based on a classical electrostatic interaction between the potassium atom and the graphite surface. Adsorption energies predicted by the electrostatic model are in good agreement with our *ab initio* calculations. In contrast, we find that the adsorption energies of potassium on carbon nanotubes are directly related to the nanotube geometry and chirality and cannot be described in terms of a simple classical model.

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