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First-Principles Studies of Ordered Potassium Monolayers on Graphite and Graphene RODRIGO B. CAPAZ, JOSUÉ X. DE CARVALHO, Universidade Federal do Rio de Janeiro, Brazil, JORGE L.B. FARIA, Universidade Federal do Mato Grosso, Brazil — We investigate the structural and electronic properties of ordered monolayers of potassium adosorbates on graphite and graphene using first-principles methods based on density-functional theory, pseudopotentials and periodic supercells. Several ordered structures are investigated and their total energies are mapped onto an effective Ising-like hamiltonian. Monte-Carlo simulations using this hamiltonian are performed in order to construct the phase diagram for this system, which is then compared to experimental results on graphite surfaces. In agreement with experiments, we find that structures with potassium concentrations larger than 1/3 ($\sqrt{3} \times \sqrt{3}$) are unstable with respect to metallic potassium segregation at the surface.

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