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Formation dynamics of graphite intercalation compounds: An *ab initio* study[1] BO SONG, HAIPING FANG, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, DAVID TOMÁNEK, Michigan State University — In response to the rising interest in functionalized graphitic nanostructures for energy applications, we study the intercalation of potassium in graphene bi-layers. Our *ab initio* molecular dynamics calculations, based on the density functional force field and simulating conditions at 900 K, provide microscopic insight into the dynamics of the intercalation process. Our model system consists of wide graphitic ribbons with hydrogenated edges and a varying number of K atoms in the unit cell. We find that following initial charge transfer from K to graphite upon adsorption, K^+ ions diffuse efficiently along the surface. After reaching the edge, K^+ ions experience further stabilization upon entering the region in-between graphene layers, accompanied by a substantial increase of the graphene inter-layer distance. We observe both intercalation and de-intercalation as competing processes in our canonical ensemble under steady-state conditions.

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