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First-principles calculations of gated adatoms on graphene¹ KEVIN T. CHAN, HOONKYUNG LEE², MARVIN L. COHEN, Dept. of Physics, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — The two-dimensional surface of graphene is well-suited for adsorption of adatoms or molecules. The application of a gate voltage can be used to precisely control the electron concentration of the adsorbate-graphene system. Such control over electronic properties of adsorbates on graphene might have useful applications in areas such as catalysis and hydrogen storage. In this work, the gating of a variety of adatoms adsorbed on graphene is studied using first-principles calculations. We compute the projected density of states, local electrostatic potential, and charge density of the adatom-graphene system as a function of gate voltage. We demonstrate that adatoms on graphene can be ionized by gating, and that the ionization causes a sharp change in the electrostatic potential. Additional interesting features of our results are also discussed.

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