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First-Principles Studies of Metal-Graphene and Metal-Nanotube Heterostructures[1] ALEJANDRO LUGO-SOLIS, IGOR VASILIEV, Department of Physics, New Mexico State University; Las Cruces, New Mexico 88003 — Metal-nanotube heterostructures have attracted considerable interest due to their potential applications in catalysis, fuel cell technology, and hydrogen storage. We investigate the optical properties of alkali metal atoms and clusters adsorbed on graphene and single-walled carbon nanotubes. The geometries, binding energies, and optical absorption spectra of the modeled structures are calculated in the framework of *ab initio* density-functional and time-dependent density-functional methods combined with the local-density approximation for the exchange-correlation functional. Our calculations show significant differences between the structures and absorption spectra of isolated alkali metal clusters and those adsorbed on graphene and carbon nanotubes.

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