Support Effects on the Catalytic Properties of Pt-Au Bimetallic Nanoparticles: A Multi-Scale Simulation Study

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Carbon nanotube-supported metal nanoparticles show promise as catalysts for a wide variety of reactions. The catalytic activity of these materials depends on their composition, structure, and the coordination numbers of exposed atoms. We have used all-atom molecular dynamics simulations to investigate the properties of bimetallic nanoparticles deposited on bundles of carbon nanotubes, focusing on nanoparticles composed of platinum and gold. The distribution of the atom types on the surface of the nanoparticle can be tuned by changing the composition of the nanoparticle and the geometry of the support. For example, it is possible to have isolated platinum atoms surrounded by gold, or chains or islands of platinum atoms. We have also used ab initio calculations to support our molecular dynamics results by studying the binding of metal atoms to carbon, and the structures of small bimetallic particles. To provide a possible link to experimental verification of our predictions, we employed ab initio DFT to investigate the adsorption of CO on selective sites identified on the adsorbed bimetallic particles.