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Understanding the Composition and Reactivity of Au/Cu Electrocatalyst Nanoparticles in Solution Using Highly Accurate Reactive Potentials[1] NONGNUCH ARTRITH[2], ALEXIE KOLPAK, Massachusetts Institute of Technology — The shape, size, and composition of catalyst nanoparticles can have a significant influence on their catalytic activity. Understanding such structure-reactivity relationships is crucial for the optimization of industrial catalysts and the design of novel catalysts with enhanced properties. In this work, we investigate the equilibrium shape and surface structure/composition of Au/Cu nanoparticles in solution, which have recently been shown to be stable and efficient catalysts for CO_2 reduction [1]. Using a combination of density functional theory calculations and large-scale Monte-Carlo and molecular dynamics simulations with reactive atomistic potentials, we determine how the nanoparticle shape, surface structure, and surface stoichiometry (i.e., fraction of Au at the surface relative to overall composition), evolve as a function of varying catalytic conditions. We discuss the effects of these changes on the surface electronic structure and binding energies of CO_2, H_2, and CH_3OH. Our results emphasize the important relationships between catalytic environment (e.g., solvent effects), catalyst structure, and catalytic activity. [1] Z. Xu, E. Lai, Y. Shao-Horn, and K. Hamand-Schifferli, Chem. Commun. 48, 5626-2528 (2012).

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