Density-Functional Theory Study of the Equilibrium Shape of Gold-Copper Nanoalloys

Nongnuch Artrith, and Alexie M. Kolpak

Department of Mechanical Engineering,
Massachusetts Institute of Technology
Cambridge Massachusetts, USA

Heterogeneous catalytic chemical reactions are at the core of many energy and environment related challenges. The shape of catalyst particles determines the accessible surfaces, and thus has a significant influence on the catalytic activity. Understanding this structure-reactivity relationship is crucial for the optimization of industrial catalysts.

Recently, Shao-Horn and coworkers have shown that gold-copper (Au/Cu) nanoparticles are stable and efficient electrocatalysts for the reduction of CO_2 to methane [1]. Our goal is to understand the structures of the Au/Cu nanoalloy at the atomic scale for further investigations of the mechanism of the catalytic reaction. Using density-functional theory, we report the equilibrium shape of Au/Cu clusters for different alloy compositions and under varying catalytic conditions.

[1] Z. Xu, E. Lai, Y. Shao-Horn, and K. Hamand-Schifferli, Chem. Commun. **48**, 5626 - 2528 (2012).