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Structure prediction of Cu-Pt nanocatalysts using a cluster expansion CHENYANG LI, TIM MUELLER, Johns Hopkins University — Electrochemical reduction of CO/CO₂ to hydrocarbon fuels can lead to a more sustainable fuel cycle. Copper and its alloys have been shown to have relatively high catalytic activities for CO/CO₂ reduction. To better understand the atomic structure and properties of Cu nanoalloys, we have generated a cluster expansion for Cu-Pt nanoparticles that enables us to rapidly predict nanoparticle energies as a function of composition, particle size and temperature. To validate and refine this approach, we have compared the predictions made by the cluster expansion to experimental characterization of Cu-Pt nanoparticles. We present a comparison of the computational and experimental results for properties including the lattice parameter, shape, and surface composition.

Chenyang Li
Johns Hopkins University

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