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Assessment of trends in the catalytic electroreduction of CO_2 on metal nanoparticles

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Metal nanoparticles are being pursued in the quest to develop more active and selective catalyst for CO_2 conversion into higher value products. Though various metal nanoparticle-based heterogeneous catalysts have shown promising electrochemical activities for reduction of CO_2, there have been no systematic studies of the reactive properties of these materials that can guide further experiments. We present large-scale screening based density functional theory (DFT) calculations to analyze trends in the activity of Ag, Au, Cu, Ir, Ni, Pd, Pt and Rh nanoparticles for CO_2 reduction. We looked at different particle size (n=13, 55, 147 and 309) to investigate its influence on the activity. Our preliminary results indicate that the relevant COOH and CHO intermediates exhibit an abnormal adsorption behavior as their adsorption strengths do not show linear correlation with that of CO. In general, the adsorption of COOH and CHO is enhanced with respect to that of CO, compared to that on the packed (111) metal counterparts. The scaling relations also were predicted to vary with system size. Based on these data, theoretical analysis of the trends in over-potentials for electrocatalytic CO_2 reduction is underway. Experimental efforts are also underway to synthesize and test variously sized nanoparticles to approximate the DFT models. Experimentally determined CO_2 reduction over-potentials and rate-limiting steps will be compared with calculated results.

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