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Research Summary:

Our current research focuses on the use of Density Functional Theory techniques to understand the kinetics and thermodynamics of chemical reactions on nanostructured metal and oxide surfaces. We aim to develop models of reactions relevant to heterogeneous catalysis and to electrocatalysis; in tandem, we will develop computational screening techniques that will permit the efficient design of new catalytic materials from first principles. Selected reactions of interest include the CO electrooxidation reaction, the selective, oxidative dehyrdrogenation of propane to propene, and the electrooxidation of small organic molecules; these reactions play an important role in the operation of fuel cells and in the production of useful chemical compounds from raw hydrocarbon feedstocks. A related interest is the development of new, first principles-based techniques to model the dissolution and corrosion of metallic surfaces; this research is related to the development both of catalysts that are stable in electrochemical environments and of corrosion-resistant surfaces.

Selected Recent Publications:

"Subnanometer Platinum Clusters: Highly Active and Selective Catalysts for Oxidative Dehydrogenation", Vajda, S., Pellin, M. J., Greeley, J. P., Marshall, C., Curtiss, L. A., Ballentine, G. A., Elam, J., Catillon-Mucheri S., Redfern, P. C., Zapol, P., Nature Materials, 8, p 213, 2009.

"Combinatorial Density Functional Theory-Based Screening of Surface Alloys for the Oxygen Reduction Reaction", Greeley, J. P., Norskov, J. K., J. Phys. Chem. C., 113, pp 4932-4939, 2009.

"Unique activity of platinum ad-islands in the CO electrooxidation reaction", D. Strmcnik, D. Tripkovic, D. van der Vliet, K. C. Chang, V. Komanicky, H. You, J. Greeley, V. Stamenkovic, and N. M. Markovic, *J. Am. Chem. Soc.*, **130** (2008) 15332.

"Voltammetric Surface Dealloying of Pt bimetallic nanoparticles: An experimental and DFT computational analysis", P. Strasser, S. Koh, and J. Greeley, *Phys. Chem. Chem. Phys.*, **10** (2008) 3670.