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Near-surface alloys for improved catalysis.

MANOS MAVRIKAKIS, UW-Madison

Periodic self-consistent Density Functional Theory (DFT-GGA) calculations have emerged as a valuable partner to experiment in explaining reactivity of transition metal surfaces. These methods provide detailed *atomic level* mechanistic information on individual elementary reaction steps, in terms of reaction thermochemistry, reaction paths, and activation energy barriers. *Trends* in reactivity derived from systematic investigations of specific steps on a number of different metal surfaces are reliable, when compared to experiment. In particular, we will attempt to demonstrate how first-principles methods can extend beyond the detailed mechanistic analysis of catalytic reactions to reach the ambitious goal of identifying promising catalysts for specific applications. Among others, we will discuss opportunities to design bimetallic catalysts for highly selective hydrogen transfer reactions, and for designing cheaper and more active oxygen reduction catalysts, the latter being most relevant to the cathode reaction of low temperature fuel cells.