

## **4a First-Principles Screening of Alloys for Heterogeneous Catalysis**

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Recent advances in Density Functional Theory (DFT) algorithms, combined with the ever-increasing availability of raw computer power, have put forth the tantalizing possibility that first-principles methods may soon contribute to the efficient screening and design of heterogeneous catalysts. For such computational design efforts to be successful, however, key catalytic parameters for the reactions of interest (binding energies, activation barriers, etc.) must be identified, and an efficient scheme for finding alloys that optimize these parameters must be developed.

In this poster, I discuss theoretical methods for the identification of critical catalytic parameters in electrochemical systems, and I demonstrate how these analyses, in concert with Density Functional Theory calculations, are used to estimate the catalytic properties of hundreds of transition metal alloys. I discuss how genetic algorithms can be used to facilitate this screening process, and I identify promising catalytic systems that might be logical targets for future investigation.