First-Principles Screening of Alloys for Electrocatalysis

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Density Functional Theory-based techniques have the potential to efficiently screen large numbers of transition metal alloys for desirable catalytic properties at relatively low cost. However, the triple challenges of identifying suitable descriptors for reactions of interest, of finding methods to efficiently determine the values of these descriptors on different metals and alloys, and of reliably estimating the stability of promising catalytic candidates in reactive environments, have generally limited the application of computational screening techniques to electrocatalytic systems.

In this talk, I describe a general methodology for electrocatalyst screening using atomic-scale simulation methods. The method employs DFT calculations to estimate important features of catalytic performance, including catalyst activity, structure, and stability, and it is applied to the analysis of hundreds of transition metal alloys for use in two reactions of interest in electrochemistry, the hydrogen evolution and oxygen reduction reactions.

References

"Computational High-Throughput Screening: New Electrocatalytic Materials for Hydrogen Evolution." J. Greeley, T. F. Jaramillo, J. Bonde, I. Chorkendorff, and J. K. Nørskov, *Nature Materials* **5** (2006) 909.