510e Large-Scale, 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 talk, we examine two methods for determining alloys with optimal catalytic parameter values: the development of exhaustive databases of parameters, useful for small populations of alloys, and the use of evolutionary algorithms, of interest for larger alloy populations. The mechanics of both methods are described, and the application of these methods to the evaluation of catalysts for an important electrochemical reaction, the oxidation-reduction reaction (ORR) in low-temperature fuel cells, is discussed.