Traversing the chemical space: Alloy catalysts discovery using Alchemy

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There is great interest in finding catalysts that do not contain precious metal catalysts. Computational quantum chemistry can be used to screen for new catalyst structures that can then be made experimentally. Unfortunately, the chemical space of alloy materials is very large and Kohn-Sham Density Function Theory (DFT) would be intractable. However, model Hamiltonian methods such as computational Alchemy [1-3] can be used to approximate the energies obtained from DFT of new structures at a small fraction of the computational cost. This poster reports our recent work on using computational Alchemy to screen the hydrogen evolution activity of 3,350 alloys based on Sabatier principle descriptors [4].

Reference:

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