

How to Find and Understand New Electrocatalysts?

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In the presentation, I will present our recent efforts to combine machine learning guided experimental studies to optimize electrocatalysts with computational investigations. It will be demonstrated how complex materials such as high entropy alloy nanoparticles can be used as a platform for catalyst discovery and understanding. One of the hypotheses of our approach is that by inverting the conventional bottom-up approach of increasing the complexity of well-defined catalysts a more efficient top-down approach can be defined. In this top-down approach, we start with complex compositions of catalysts and continuously tune their constituent components do down select to optimal materials.

Based on examples, the merits of this approach as well as the challenges are discussed.
