Learning in Higher Dimensions: A Strategy for Alloy Catalyst Discovery

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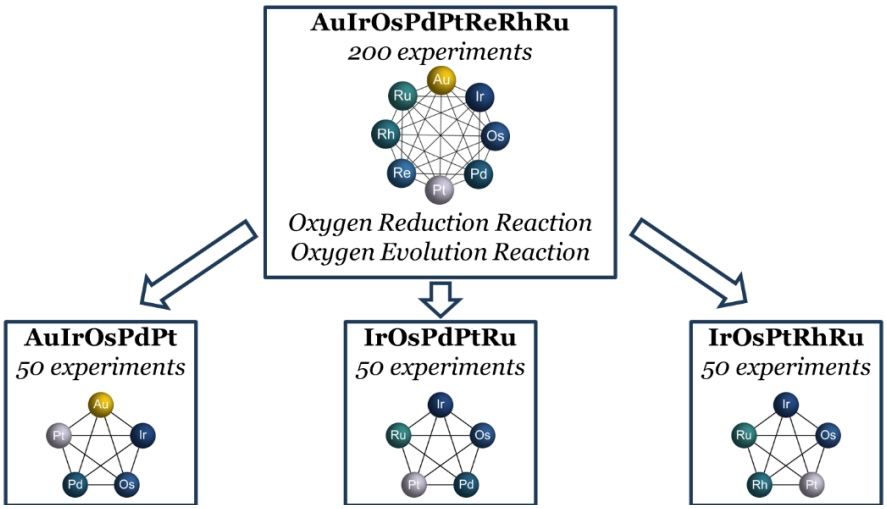
In the last couple years, the topic of high entropy alloy (HEA) catalysts gained increased attention.1 Composed of 5 elements or more, the number of possible HEA catalysts reaches astronomically large numbers. As such, statistical approaches are required to efficiently study HEA catalysts. In our previous works, we investigated the benefits of using Bayesian optimization to search a HEA composition space for the most active HEA catalyst.2,3 In parallel, we have seen the strengths of machine learning models to investigate correlations in the HEA composition spaces themselves. Lately, we have demonstrated that studying HEA catalyst composition spaces is more effective by including as many as possible elements in a single study.4 With this idea, we have studied the AuIrOsPdPtReRhRu composition space for the oxygen reduction reaction and oxygen evolution reaction. This was achieved by synthesizing 350 nanoparticles and training machine-learning models with the acquired data. These machine learning models, showed high resilience to outliers which strengthens the validity of the models. Lastly, the combination of DFT calculations with machine learning models provides a comparison of catalytic trends across a complete composition space and thus an advanced test to their predictive power.



1. Löffler, T., Ludwig, A., Rossmeisl, J. & Schuhmann, W. What Makes High-Entropy Alloys Exceptional Electrocatalysts? Angewandte Chemie - International Edition vol. 60 26894–26903 Preprint at https://doi.org/10.1002/anie.202109212 (2021).
2. Pedersen, J. K. et al. Bayesian Optimization of High-Entropy Alloy Compositions for Electrocatalytic Oxygen Reduction**. Angewandte Chemie - International Edition 60, 24144–24152 (2021).
3. Mints, V. A. et al. Exploring the Composition Space of High-Entropy Alloy Nanoparticles for the Electrocatalytic H2/CO Oxidation with Bayesian Optimization. ACS Catal 12, 11263–11271 (2022).
4. Mints, V. A., Pedersen, J. K., Wiberg, G. K. H., Rossmeisl, J. & Arenz, M. Backward Elimination: A Strategy for High-Entropy Alloy Catalyst Discovery. doi:10.26434/chemrxiv-2022-78s83.