Center for High Entropy Alloy Catalysis' highlights in 2021:

Catalysis is key in the future development of, and transition to green chemistry and the renewable production of chemicals and fuels. However, this transition requires new catalysts, as central chemical reactions cannot be catalysed with existing materials. The challenge is to discover new catalyst materials, which are both stable and active. There are basically infinitely many possible High Entropy Alloy materials which are yet to be discovered. However, we need to develop intelligent ways of searching the space of HEAs and identify the interesting alloys among all the rest.
[What Makes High-Entropy Alloys Exceptional Electrocatalysts?, Angewandte Chemie, 2021 - https://doi.org/10.1002/anie.202109212]

Imagine an alloy consisting of five different elements; stepping this alloy in 5% fractions would lead to more than 10.000 possible materials with different compositions, see figure. This number of compositions is impossible to test experimentally, and hence we have developed a search algorithm in the HEA composition space to quickly find the most promising catalysts.
The algorithm suggests a sample for a new composition based on the data from the previous sample and with the new result, the algorithm updates its understanding of the space and suggests a new composition to test. We observed that within a set of only 50 compositions the algorithm has found the most active catalysts. The activity of the 50 compositions are estimated by simulations. However, we tested the most promising alloys experimentally and confirmed that their activities are indeed higher than for the pure elements. Some of these catalysts have previously been suggested in literature, others have not.
[Bayasian Optimazation of High-Entropy Alloy Compositions for Electrocatalytic Oxygen Reduction, Angewandte Chemie, 2021 - https://doi.org/10.1002/anie.202108116]

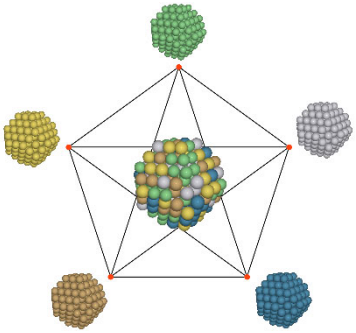

Figure: An illustration of the 4D composition space for an alloy consisting of five different elements. The HEAs in the middle haven't been investigated yet, meaning that there are a huge unknown chemical space for discovering new catalyst materials.

This gives hope that we, with a limited number of real experiments, in the future can search the multi-dimensional space of a high entropy alloys and discover the interesting catalysts.

We have started to compare theory (simulations) and experiments of the catalysis on high entropy alloy surfaces. There hasn't been combined simulation and experimental studies, up until now. Our external collaborators can make materials where the composition gradually change over a disk. The disk is made from five sources of pure metals and the composition at a spot depends on the distance to all the different sources. Furthermore, they perform high throughput screening of the catalytic activity over the many different compositions at the disk in parallel and compare with our simulations. The combination of parallel screening and simulations is close to ideal for understanding trends and can thereby reveal relationships between the composition and the activity.
[Complex-Solid-Solution Electrocatalyst Discovery by Computational Prediction and High-Throughput Experimentation, Angewandte Chemie, 2021 - https://doi.org/10.1002/anie.202014374]

Even with the high throughput screening, only a tiny fraction of the possible compositions are experimentally tested, therefore the predictions from simulations are needed to understand and search the entire composition space.