Center for High Entropy Alloy Catalysis' highlights from 2022:

Danish National Research Foundation offers a fantastic opportunity for a newly established Center of Excellence to organize and host a conference, within the center's field of research, with additional funding. We had the pleasure of hosting a DNRF conference on High Entropy Electrocatalysis in May 2022, at Bella Sky Conference & Hotel. We had 80 participants from around Europe.
It was just after the pandemic and the field of High-Entropy Alloys is very young, and so, it was the first time that many of the participants met in real life. This applied both for young and more senior scientists. Even some of our collaborators from Bochum, we met off-line for the first time, in spite of several joint published articles. It is just much more inspiring to meet in the physical world. There were very inspiring talks, all related to high entropy alloys and catalysis. We had talks from leaders in the field combined with talks from post docs and PhD-students. Our 'own' post docs and students represented CHEAC and the research we do, either by talks or at the poster session. Post doc Andrea Kirsch from UCPH won the "Best Poster" prize.

Photo: Jens-Christian Navarro Poulsen

Research:

Imagine an alloy consisting of four different elements and think of the composition space representing all different possible ratios between these elements, see the figure.
The corners represent the pure elements, the edges the binary, facets are the trinary alloys, and the bulk are alloys including all four elements. By including a fifth element, the space becomes 4-dimentional. The task is to explore this space and find the most promising catalyst materials. However, without a search strategy it is difficult to find the interesting areas in this space. A given point in the space will correspond to a measurement of activity for a specific composition. In 2021, we developed a search-algorithm in the HEA composition space to find the most promising catalysts fast, based on Bayesian Optimization on top simulations. The conclusion was that based on simulations, approximately 50 experiments of different compositions, should be sufficient to explore and exploit a composition space of five elements.

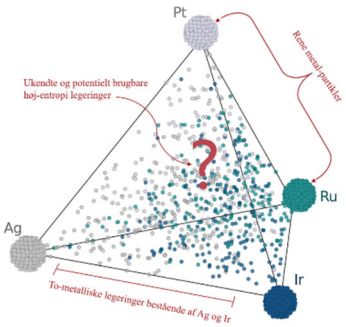

Figure by Christian M. Clausen

In 2022, we used this method with experiments, which further supported that it is actually relatively few experiments that are needed to explore the space. This suggests that medium throughput experimentation is sufficient to explore the space in this case. This work is the first comparison, between theory and experiments, all done within CHEAC. [Exploring the Composition Space of High-Entropy Alloy Nanoparticles for the Electrocatalytic H2/CO Oxidation with Bayesian Optimization, VA Mints, JK Pedersen, A Bagger, J Quinson, AS Anker, KMØ Jensen, J Rossmeisl, M Arenz, ACS Catalysis 12 (18), 11263-11271, 2022]