Center for High Entropy Alloy Catalysis' highlights from 2023

Summer school: Many researchers consider summer schools their highlights of the year. At these events, the presentations tend to be longer, more inspiring, and more educational compared to those at conferences. The venues are often a nice, remote location, difficult to get to and from. Therefore, students have the opportunity to meet researchers who share the same passion and talk to some of the "scientific rock stars", discovering that they are approachable.

We hosted a four-day summer school on High Entropy Materials in August 2023 at Metalskolen in Jørlunde. Approximately 65 participants from various countries attended. The program commenced with an inspiring keynote address by Brian Cantor, one of the pioneers in High Entropy Alloys. Talks were delivered by both senior and emerging researchers from the US, India, and Europe, embodying the essence of what a summer school should be. Our aspiration is that this event will remain a cherished memory for the students, just as it has been for us.

Research:

The more the better: on the formation of single-phase high entropy alloy nanoparticles as catalysts for the oxygen reduction reaction
Rebecca K. Pittkowski, Christian M. Clausen, Qinyi Chen, Dragos Stoian, Wouter van Beek, Jan Bucher, Rahel L. Welten, Nicolas Schlegel, Jette K. Mathiesen, Tobias M. Nielsen, Jia Du, Asger W. Rosenkranz, Espen D. Bøjesen, Jan Rossmeisl, Kirsten M. Ø. Jensen and Matthias Arenz. **EES. Catal., 2023, 1, 950-960.**

This work exemplifies a collaborative endeavor within CHEAC, integrating synthesis, characterization—including both diffraction and microscopy—and simulations to unravel the formation mechanisms of HEA nanoparticles.
Conventional methods for producing HEA materials typically involve high temperatures and controlled cooling rates, often resulting in particles that are too large for effective catalysis. In the work, we explored low-temperature synthesis strategies for alloying five different noble metals. Employing advanced diffraction and microscopy techniques, we have confirmed the randomness of the elements in the particles. Our findings reveal that stochastic events play a pivotal role in this process, demonstrating that systems with a greater number of atom types and limited atom mobility during the synthesis are more predisposed to form random alloys.
This study underscores the significance of comprehending formation mechanisms to devise innovative, low-temperature approaches for efficiently synthesizing small HEA nanoparticles.

A Flexible Theory for Catalysis: Learning Alkaline Oxygen Reduction on Complex Solid Solutions within the Ag–Pd–Pt–Ru Composition Space.
Christian M Clausen, Olga A Krysiak, Lars Banko, Jack K Pedersen, Wolfgang Schuhmann, Alfred Ludwig, Jan Rossmeisl, Angewandte Chemie International Edition 62 (39), e202307187.

This collaborative effort involved two research groups in Bochum, with whom we have cultivated a highly productive partnership over the past 4-5 years. The primary objective of this paper was to derive a theoretical model for a reaction directly from experimental data. We presented an approach to achieve this by comparing high-throughput experiments with calculations. Our findings indicate that the theoretical model we previously developed for the reaction (ORR) stands out as one of the most effective models in representing the data. Additionally, our comparison suggests that the measured composition of the HEA film does not always align with the composition that would yield the best fit between theory and experiments. This implies that we first utilize experiments to elucidate the theory for the reaction, and subsequently employ the theory to gain insights into the experimental structures.