

Center for High Entropy Alloy Catalysis' highlights in 2020:

We aim to discover new catalyst materials for a series of energy conversion reactions for the future; oxygen reactions, hydrogen reactions and other Power-To-X reactions.

Assistance to the green transition?

The commercialization of green hydrogen fuel cells depends on efficient and stable electrocatalysts. For fuel cells, hydrogen and oxygen are separately converted at the cathode and anode to give the overall reaction. The majority of improvement is to be made for the oxygen reduction reaction, which is the limiting factor to improve efficiency.

Today's catalysts for the oxygen reduction reaction are based on platinum-cobalt nanoparticles supported on carbon materials. The nanoparticles ensure a large catalytic surface area, allowing the most of the expensive platinum atoms to be a part of the surface - where the catalysis takes place. The supported carbon material has the feature to ensure electronic contact to the nanoparticles and a high surface area. Unfortunately, the carbon material is vulnerable to corrosion which limits the lifetime and operation conditions of fuel cells.

Publication:

We have discovered, a new carbon-free concept consisting of self-supported networks of nano-wires of platinum-cobalt that combines high intrinsic activity with unprecedentedly high catalytic surface area and conductivity within the nanowires.

The work was published in Nature Materials and it is a highlight for CHEAC as it is the first joint paper between all the centre's PIs. This work was also highlighted in the press by DR (<https://www.dr.dk/nyheder/viden/teknologi/er-brint-fremtiden-dansk-bil-teknologi-kan-goere-brintbiler-billigere>), Berlingske (<https://www.berlingske.dk/videnskab/har-koebenhavns-universitet-banet-vejen-for-brintbilens-gennembrud>) and Der Spiegel (<https://www.spiegel.de/auto/brennstoffzelle-neuer-katalysator-soll-kosten-deutlich-senken-a-c6b95652-6333-4f49-ae6c-d43a1e698953>).

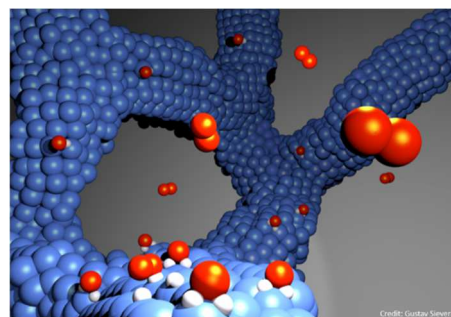


Illustration of a network of nano-wires: The high surface area is achieved by the platinum-cobalt bone nanostructure and the nano-wires are conducting themselves so the carbon material is not needed for electronic contact.

Another path in the green transition

CO₂ reduction to carbon hydrides is one of the corner stone reactions for Power-to-X, as it is a way of closing the carbon cycle and make fuel out of CO₂. Among the pure metals, only Copper (Cu) can catalyse that reaction, but not in a selective manner.

We utilized a statistical approach through computer simulations to discover new multicomponent alloys that could show some of the same properties as copper. Our results show several promising alloys, some of which were already known in the literature, which ensures our theory and understanding of the reaction. However, it is still too early to say if they have better properties than copper.

This work was our first work on High Entropy Alloy Catalysis after the start of CHEAC. It was published in *ACS-catalysis* and it has already been cited many times.