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Operando stability investigation of ORR electrocatalysts

Hydrogen fuel cell

Hydrogen fuel cells are key part in the process of decarbonization of electricity production as the fuels are hydrogen & oxygen and the products are electricity & water.

Proton Exchange Membrane Fuel Cell (PEMFC) is a variant that uses a ionic membrane as a solid electrolyte conducting protons only. On the anode side of the membrane a Hydrogen Oxidation Reaction takes place and on the cathode side a **Oxygen Reduction Reaction** (ORR) occurs.

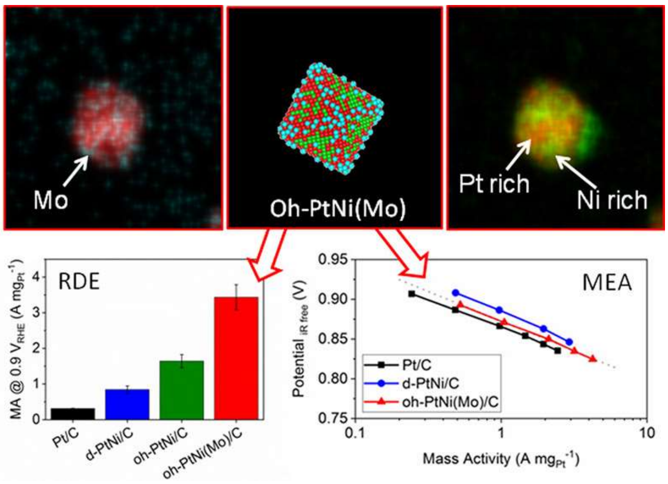
Due to the high gravimetric energy density (33 kWh/kg) of hydrogen in comparison to Li-ion batteries (0.2 kWh/kg), PEMFC are being used not only for stationary electricity generation, but also to power engines of electro vehicles where a high current throughput is needed.

What is the industrial problem?

ORR is the main bottleneck limiting the maximum current density produced by a hydrogen fuel cell. The activity depends strongly on the surface structure of the catalyst and thus, a great deal of research is being done to carefully tune the catalyst shape to overcome sluggish ORR kinetics.

One promising approach is to create octahedra (oh) platinum alloy nanoparticles (NPs). Oh-PtNi(Mo) catalysts show an exceptional improvement in the mass activity for conventional **rotating disc electrode** (RDE) screenings in electrolyte[1]. However, in a **membrane electrode assembly** (MEA), the heart of a real hydrogen fuel cell device, the high performance enhancement vanishes.

Compare **3.43 A/mg$_{Pt}$** in RDE vs. **0.45 A/mg$_{Pt}$** in MEA.



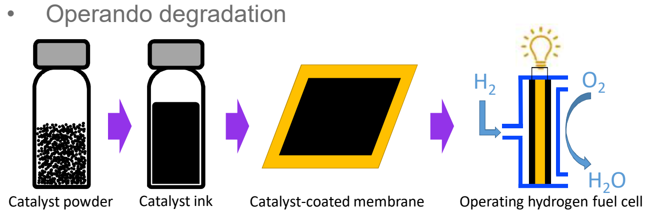
Identifying the imposter

There are two main steps in the transition from a fresh catalyst in RDE to the operating MEA in a fuel cell that might contribute to the decreased activity:

- Ink preparation
- Membrane manufacturing

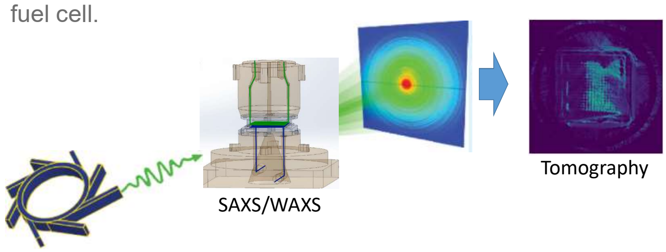
In addition, conditions under which the fuel cell operates have a high impact on catalyst long term performance.

- Operando degradation



Tackling the issue

In this project, we will synthesize advanced shape-controlled Pt alloyed catalysts. Using Small and Wide Angle X-ray Scattering techniques (SAXS, WAXS), we will track down the degradation from the fresh catalyst through the ink preparation to various operation conditions in a custom 5 cm^2 fuel cell.



Where SAXS gives us the information on changes in particle sizes, shapes and interparticle distance, WAXS provides information about crystallinity and microstrain that shows a direct link with the catalytic activity[2]. In combination with operando tomography, we are able to see inside the fuel cell and corelate the influence of the whole system with structural changes of the catalyst and with the overall performance.

What are the expected outcomes?

1. Obtaining a complex understanding of the processes that leads to the activity depression of the catalyst in the transition from a fresh powder to the MEA in the PEMFC.
2. Identify ideal conditions for high current density operation of advanced oh-Pt-alloyed NPs in a hydrogen fuel cell.

References

(1) Dionigi, F. et al. (2019). Controlling Near-Surface Ni Composition in Octahedral PtNi(Mo) Nanoparticles by Mo Doping for a Highly Active Oxygen Reduction Reaction Catalyst. *Nano Letters*, *19*(10), 6876–6885. https://doi.org/10.1021/acs.nanolett.9b02116

(2) Chattot, R. et al. (2018). Surface distortion as a unifying concept and descriptor in oxygen reduction reaction electrocatalysis. *Nature Materials*, *17*(9), 827–833. https://doi.org/10.1038/s41563-018-0133-2

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