

Annual meeting of the COST Action:

Computational materials sciences for efficient water splitting with nanocrystals from abundant elements (CA18234)

“Computational water splitting, where we are now and where to go?”

Oxygen Evolution Reaction with IrO₂ and IrO₂-based hybrid materials

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H₂ production through water electrolysis is a very promising strategy for storing sunlight energy. For the limiting oxygen evolution reaction, iridium oxide containing materials are very promising due to their stability in acidic conditions. Unfortunately, iridium is an expensive precious metal and thus, lowering the iridium content on the catalyst is an essential issue for their practical implementation. Several research groups have synthesized small IrO₂(IrO_x) nanoparticles of about 1.5 – 2.0 nm that have been shown to be within the most active species, particularly when normalizing by the catalyst amount. Indeed, the ultimate goal is the use of atomically dispersed iridium centers which allows optimizing the noble metal content and the number of active sites. In this context, several single atom catalysts (SACs) containing iridium have been shown to catalyze the OER reaction with low overpotentials and high catalytic activities.

In this contribution, we will present our recent results on the catalytic activity for the oxygen evolution reaction of iridium-based materials focusing on extended surfaces, nanoparticles and single atom catalysts. For each type of material, we will cover the model construction (particularly for the case of nanoparticles), the material-water interface and the catalytic process itself. Results show that low coordinated sites particularly at corner and tip sites of the nanoparticle or acting as single atom catalysts are not fully oxidized at reaction conditions and show slightly higher catalytic activities.