

## Earth-abundant nano-catalysts for clean hydrogen fuel generation through water splitting

Junyuan Xu

### Abstract

Hydrogen (H<sub>2</sub>) has been proposed to be a clean and carbon-neutral energy carrier that can be used as next-generation fuel to fulfill both stationary and transportation needs. Compared to steam reforming, electro-catalytic water splitting represents a greener and more sustainable way for H<sub>2</sub> generation and has been intensively investigated in recent years. The Oxygen Evolution Reaction (OER) has been a bottleneck to improve water splitting efficiency. It involves four concerted proton-coupled electron transfer steps and is both thermodynamically and kinetically demanding. Without a catalyst, the OER usually takes place at a high over-potential leading to a large energy loss. Compared to the OER, the H<sub>2</sub> Evolution Reaction (HER) can be accomplished comparatively easily, but efficient electro-catalysts are still needed to reduce the over-potential for HER and enable the reaction to take place at a practically high rate. Lately, earth-abundant transition metal based electrocatalysts have been demonstrated to be highly active for both HER and OER and are proposed to be promising alternatives to Platinum Group Metal (PGM) catalysts for use in water electrolyzers. In this study, we showed our recent efforts to developing efficient and durable transition metal based electrocatalysts, including transition metal phosphides obtained by wet chemical reduction followed by post-phosphorization treatment and cobalt ultrafine clusters prepared by cluster beam deposition. We have demonstrated that all these catalysts show electro-catalytic performance favorably compared to PGM based electrocatalysts for HER or OER and therefore hold substantial promise for use as low-cost catalysts in water electrolyzers.

Electrocatalytic water splitting is a promising approach to generating hydrogen from water. In order to enhance water splitting efficiency, it is essential to promote gas revolution from catalysts surface, reduce the over-potential of oxygen evolution (OER), and inhibit the production of the hydrogen peroxide by-product. To realize them, in this work, we take a cue from nature to promote water splitting activity of hollow porous Fe<sub>3</sub>O<sub>4</sub> microspheres (M – Fe<sub>3</sub>O<sub>4</sub>) with the aids of hemoglobin. Hemoglobin monolayer was self-assembled on

the surface of M – Fe<sub>3</sub>O<sub>4</sub> catalysts. It transported newly-generated oxygen molecules away from catalysts surface and exhibited chiral-induced spin selectivity (*CISS*) effect during OER reaction. Owing to the “helping hand” of hemoglobin, the OER onset potential of hollow porous Fe<sub>3</sub>O<sub>4</sub> microspheres reduced by 100 mV and the current density was enhanced 2 folds. The results indicate a new strategy for designing earth-abundant catalysts which combine the merits of oxygen transferring and *CISS* effect for electrocatalytic water splitting.

### Biography

Junyuan Xu has completed his PhD degree from University of Science and Technology Beijing (USTB) in January 2014 with a thesis entitled “High performance oxygen evolution reaction catalyst in acid for Proton Exchange Membrane (PEM) water electrolysis”. During his PhD study, he has worked as a Scientific Visitor at Technical University of Denmark (DTU) for one year. In March 2014, he became a Post-doctorate Fellow at the Catalysis and Materials Division (CMD) of the Institute of Metal Research (IMR), Chinese Academy of Sciences, under the supervision of Professor Dangsheng Su, where his research focused on electrocatalytic mechanisms of carbon dioxide conversion using heteroatom doped nanocarbon electro-catalysts. He has joined Dr. Lifeng Liu’s group at the International Iberian Nanotechnology Laboratory (INL) and is currently working as a Research Fellow on a Horizon 2020 project (CritCat) focusing on developing non-precious earth-abundant electro-catalysts for hydrogen/oxygen evolution reactions.

Junyuan Xu

International Iberian Nanotechnology Laboratory, Portugal