Universitat Autònoma de Barcelona

Selective Oxidation Catalysis (SelOxCat)
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SelOxCat Selective RedOx Catalysis

PhD Fellowship in Redox Catalysis for Artificial Photosynthesis

The *SelOxCat* Research Group at the Autonomous University of Barcelona (UAB) offers **one PhD Fellowship** (3 years) starting next September 2023.

Our Group focuses its attention on the tailored design of tunable molecular-material hybrids at the nanoscale for the cost-effective generation of H_2 and liquid carbon-neutral fuels. For further information, please visit the website: http://www.seloxcat.wordpress.com

*PROJECT: "***Tailored Catalytic Nanomaterials for the Production of Solar Fuels and Value-Added Chemicals"**: Redox catalysis is at the core of artificial photosynthetic schemes based on the splitting of water or the reduction of anthropogenic CO_2, and is thus a key area for enabling the required shift to a more sustainable future. Thus, the sustainable generation of either H_2 from water or liquid C-neutral fuels and value-added chemicals from atmospheric CO_2 relies on the development of cost-efficient and durable (photo)catalytic systems for transformations such as the hydrogen evolution reaction (HER), the oxygen evolution reaction (OER) and the CO_2 reduction reaction (CO_2RR), which is the focus of this PhD thesis. As a balance between ruggedness and cost-efficiency is sought, nanoparticulate metal/metal-oxide catalysts and (photo)electrodes are our choice. In particular, we pay special attention to their tailoring and fine-tuning, two of the main challenges still to overcome in order to attain faster kinetics and higher selectivities with heterogeneous catalytic species. In this regard, following our approach based on the surface-functionalization of metal/metal-oxide nanoparticles[1] we will explore, 1) the role of capping ligands in the activity and reaction mechanisms of surface-functionalized nanocatalysts through a combined experimental/computational approach, 2) the impact of introducing a second metal through bimetallic alloys and single-atom-decorated nanoparticles, 3) strategies to improve the durability and cost-efficiency of (photo)electrodes based on diminishing nanoparticle aggregation under catalytic conditions and increasing the exposure of active sites, and 4) the fine-tuning of the linkage between photoabsorber molecules/materials and nanocatalyts in order to tailor electron-transfer rates and minimize charge recombination.

The candidates must hold a BSc degree in Chemistry, Nanotechnology or Materials Science and a MSc degree (or be currently pursuing it) in the same fields. High oral and written communication skills in English are required. The selected student will be awarded a 3-years contract and is expected to conduct research, write drafts of scientific papers and deliver a PhD thesis.

Interested candidates please contact **Dr. Xavier Sala** (xavier.sala@uab.cat) by email.

[1] (a) *ACS Catal.* **2018**, 8, 11094-11102. (b) *Sust. Energy & Fuels* **2020**, 4, 4170, (c) *ChemSusChem* **2019**, 12, 24943, (d) *Catal. Sci. Technol.* **2020**, 10, 4513-4521, (e) *Mater. Today Energy* **2018**, 9, 506-515, (f) Renew. Energy **2021**, 168. 668-675, (g) *J. CO_2 Util.* **2021**, 50, 101574. (h) *Dalton Trans.* **2022**, 51, 731, (i) *Adv. Energy Mater.* **2023**, DOI: 10.1002/aenm.202300282.