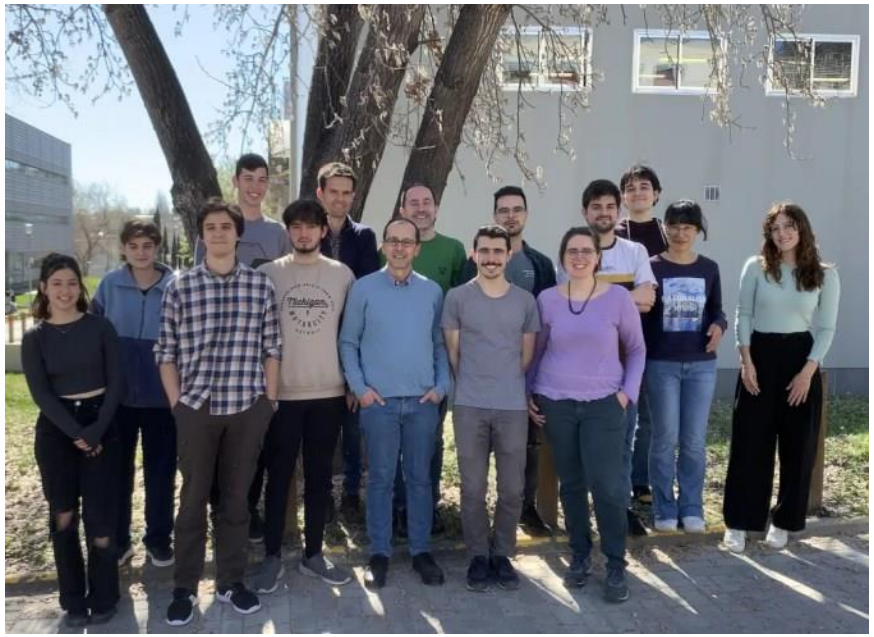
Selective RedOxCatalysis (SelOxCat) Group - UAB



Dr. Roger Bofill – UAB
Roger.Bofill@uab.cat

Dr. Jordi García Antón – UAB
Jordi.GarciaAnton@uab.cat

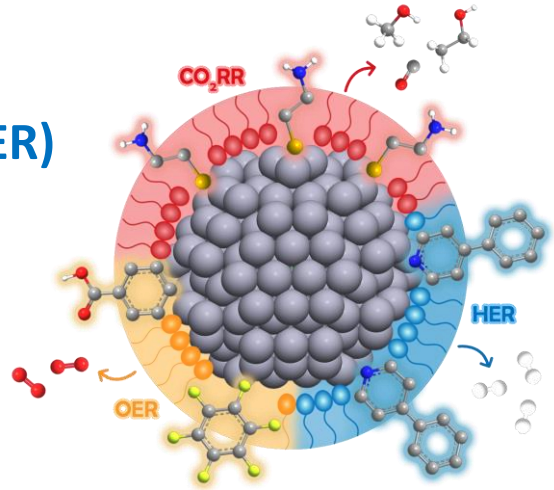
SelOxCat
Selective RedOx Catalysis

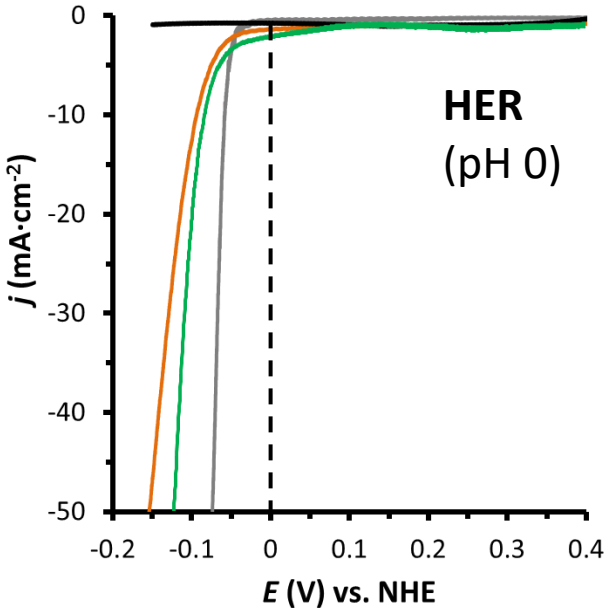
2021 SGR 00095

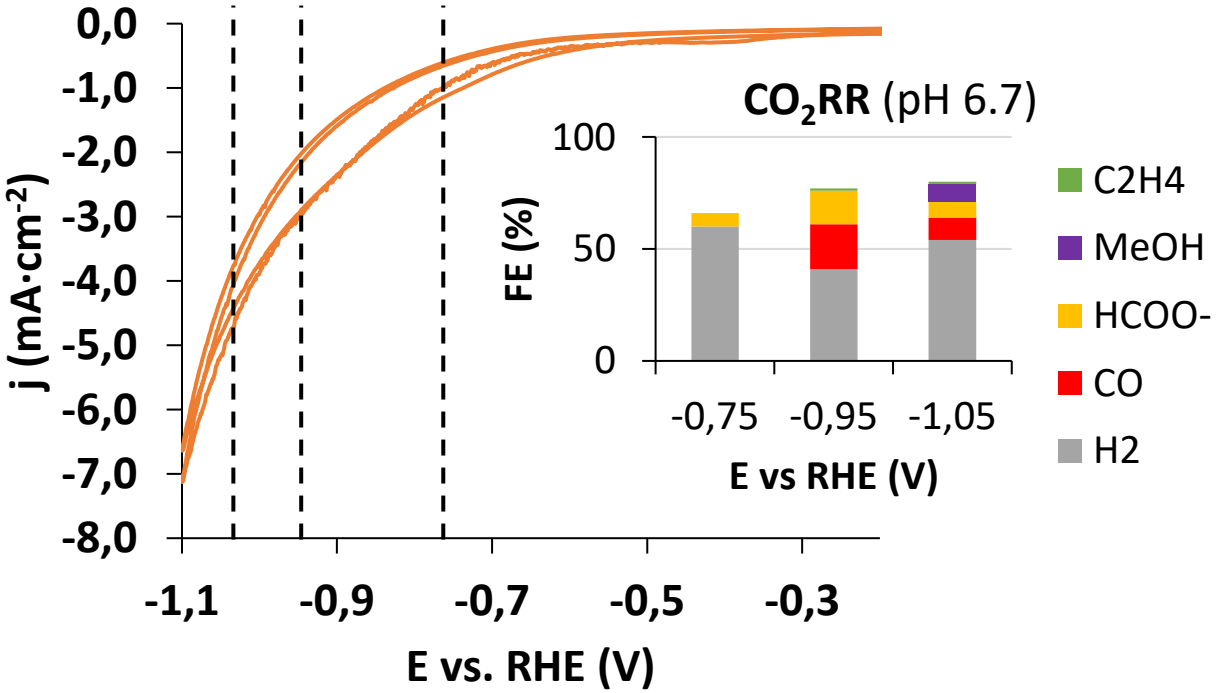
Permanent members (SelOxCat):
Dr. Xavier Sala (IP1, Associate Professor, ICREA Academia 2020)
Dr. Jordi García-Antón (IP2, Associate Professor)
Dr. Roger Bofill (Associate Professor)
Dr. Lluís Escriche (Associate Professor)
Dr. Laia Francàs (RyC)
Dr. Jose Muñoz (RyC)

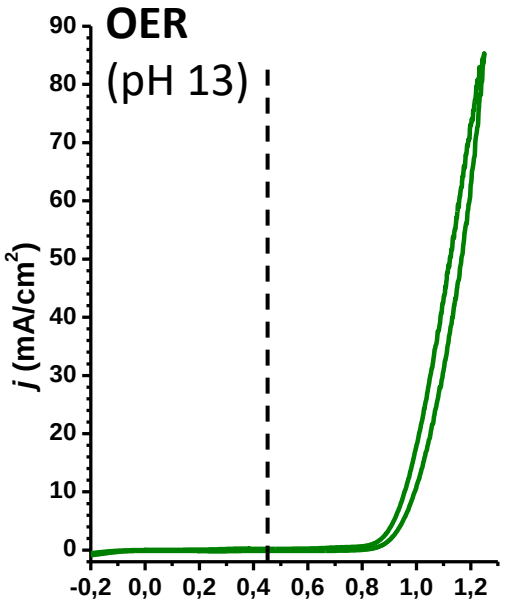
(Photo)electrocatalytic catalysis with surface-functionalized NPs

- Water oxidation (Oxygen Evolution Reaction, OER)
- Proton reduction (Hydrogen Evolution Reaction, HER)
- CO_2 reduction reaction (CO_2RR)





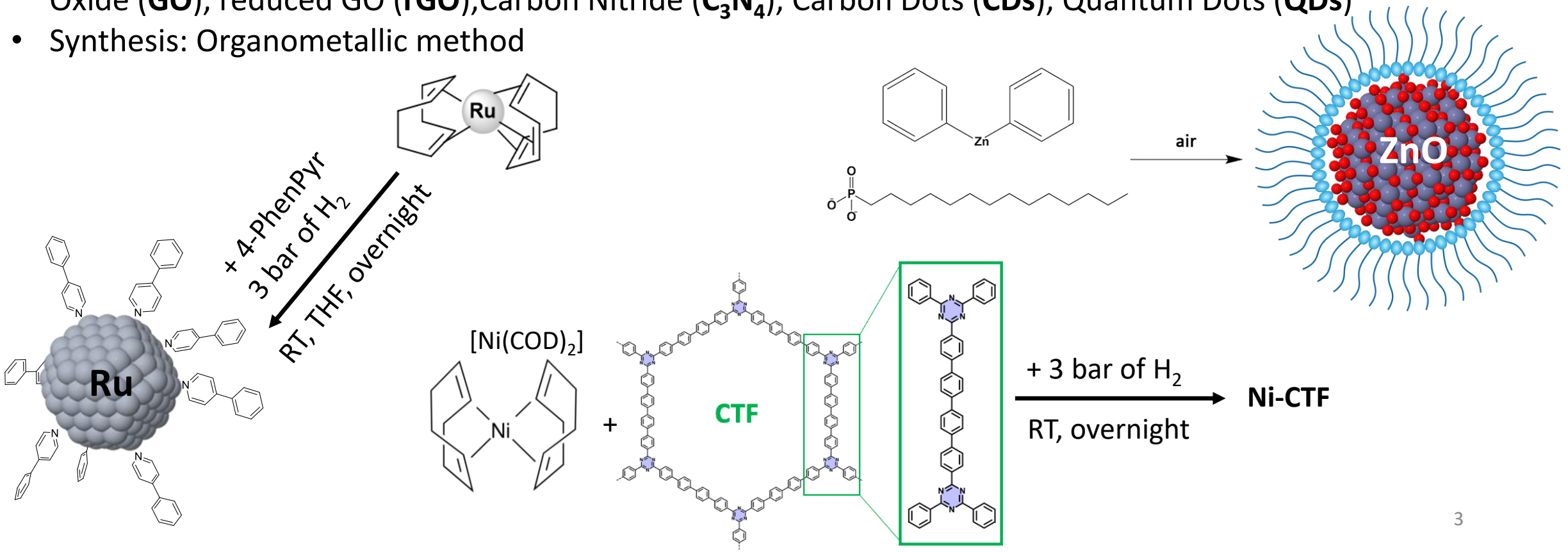




E (V) vs NHE at pH 13

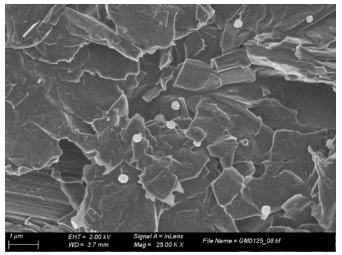
Nanoparticles (NPs) as catalysts

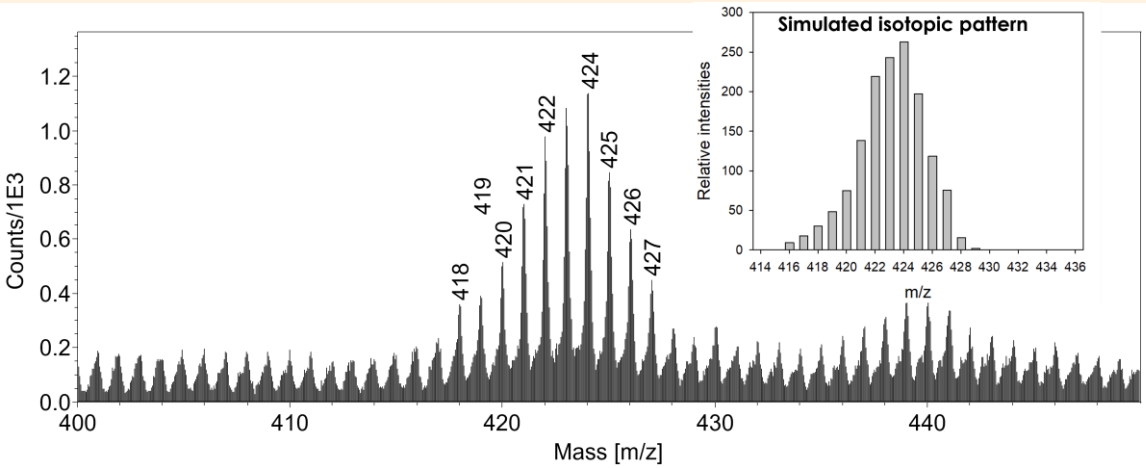
- Monometallic NPs: Ru, Co, Ni, Cu, Pt, Au, Cu, Cu_2O, ZnO, SnO_x, La, Mo
- Bimetallic NPs: Ru-Co, Ru-Pt, Ru-Ni, Cu-Zn
- Supported onto Glassy Carbon (**GC**), Fluorine-Tin Oxide (**FTO**), **TiO_2**, FTO-TiO_2, FTO-Nafion, TiO_2-Rutile, Carbon Paper (**CP**), Ni foam, Carbon Nanotubes (**CNTs**), multiwalled CNTs (**MWCNTs**), Metal Organic Frameworks (**MOFs**), Covalent Organic Frameworks (**COFs**), Covalent Triazine Frameworks (**CTFs**), Graphene Oxide (**GO**), reduced GO (**rGO**),Carbon Nitride (**C_3N_4**), Carbon Dots (**CDs**), Quantum Dots (**QDs**)
- Synthesis: Organometallic method

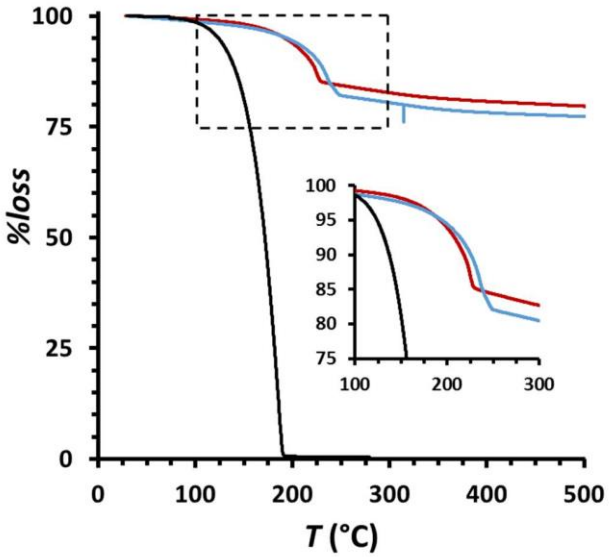


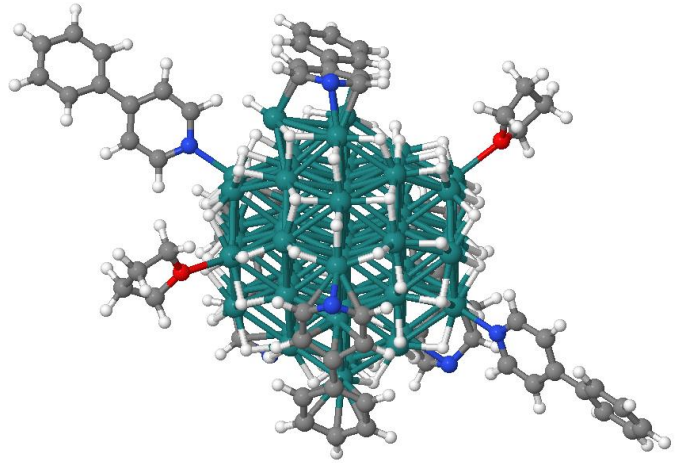
Characterization techniques

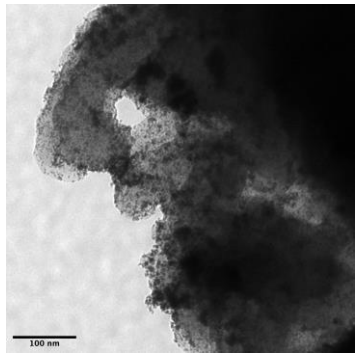
- SEM, TEM & HR-TEM, **STEM-HAADF, APT**
- TGA, ICP-OES, EA
- Cyclic Voltammetry, DPV, LSV
- Spectroelectrochemistry
- UV-Vis, IR, ATR-IR, Raman, Fluorescence, TAS
- Solution & Solid State NMR
- XPS, EDX, WAXS, **XANES**, **FT-EXAFS**
- MS, ToF-SIMS
- GC, Clark Electrodes (H_2,O_2), manometry
- DFT calculations

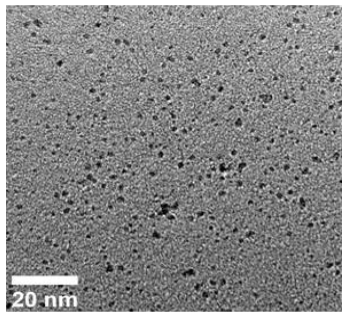


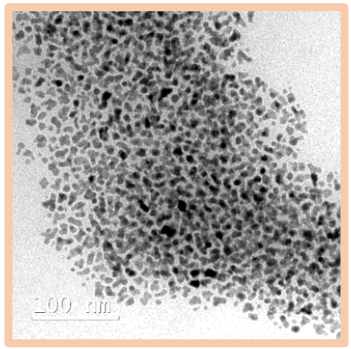








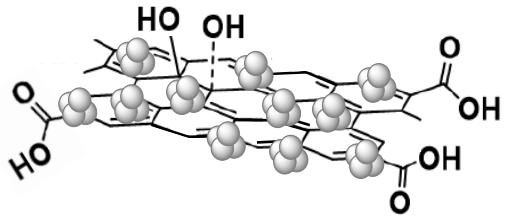




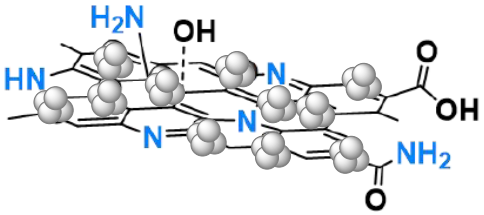
Selected examples

Supported Ru NPs on reduced Graphene Oxide for electrocatalytic HER

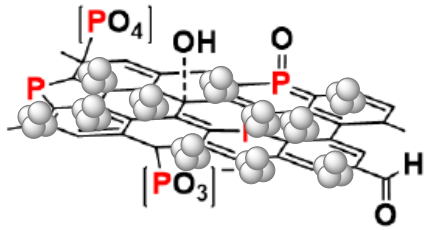
rGO (1)



N-doped rGO (2)



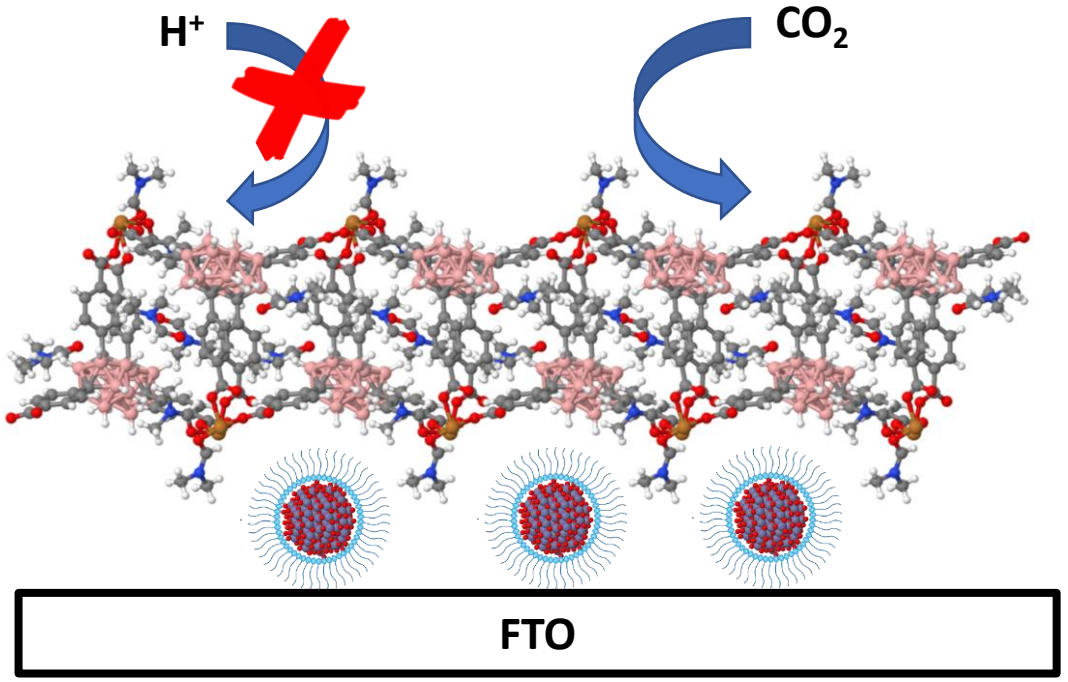
P-doped rGO (3)



Entry	System	η_{10} (mV)
1	Ru@rGO	71
2	Ru@NH_2-rGO	30
3	Ru@P-rGO	2

In collab. with **Dr. Luis Miguel Martínez Prieto** (U. Sevilla); DFT calculations in collab. with **Prof. Romuald Poteau** (UPS, Toulouse)

ZnO NPs on Cu-MOF@FTO for electrocatalytic CO_2RR

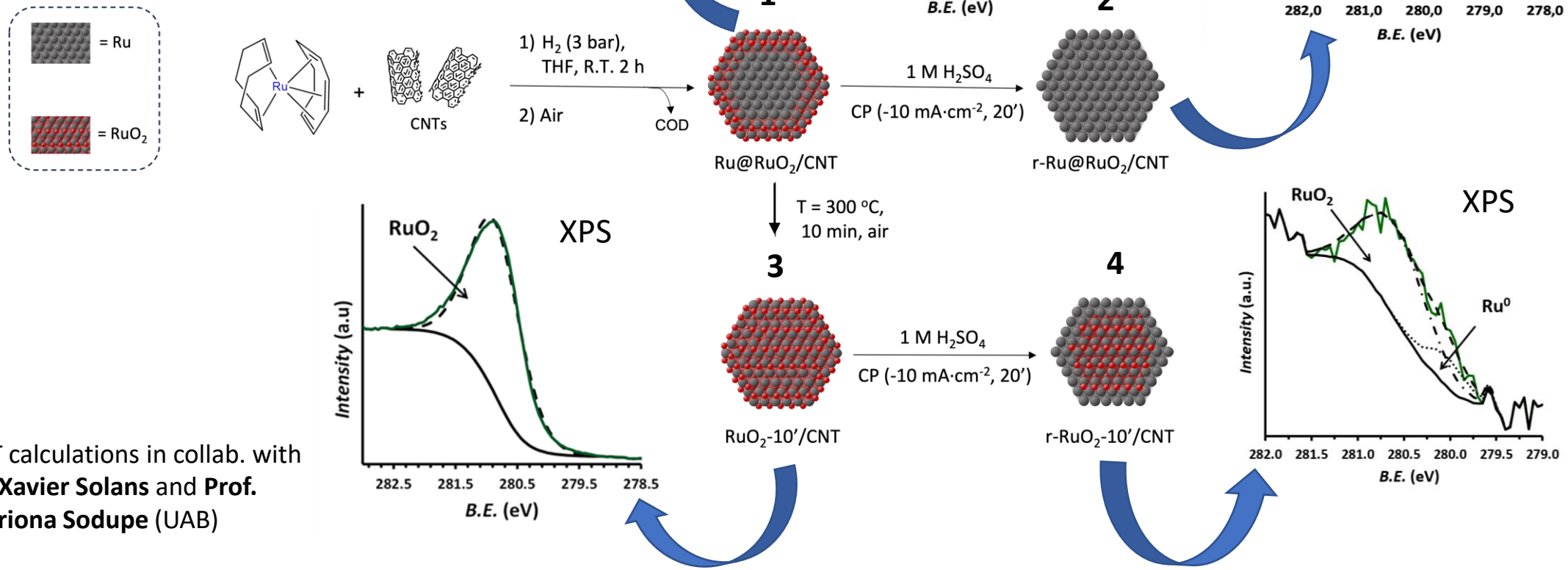


In collab. with **Dr. José Giner Planas** (ICMAB-CSIC)

Selected examples

Ru/RuO_2 core/shell NPs supported on CNTs for electrocatalytic HER

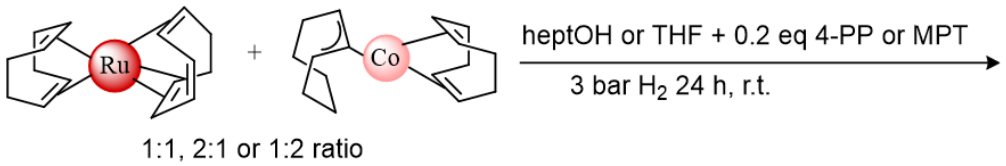
Entry	System	NP composition	η_0 (mV)	η_{10} (mV)
1	$Ru@RuO_2/CNT$	Ru/RuO_2 core/shell	200	272
2	$r\text{-}Ru@RuO_2/CNT$	Ru^0	150	222
3	$RuO_2\text{-}10'/CNT$	RuO_2	130	319
4	**$r\text{-}RuO_2\text{-}10'/CNT$**	**RuO_2 /Ru core/shell**	**50**	**115**

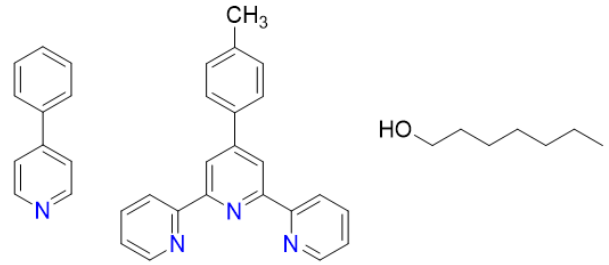


DFT calculations in collab. with **Dr. Xavier Solans** and **Prof. Mariona Sodupe** (UAB)

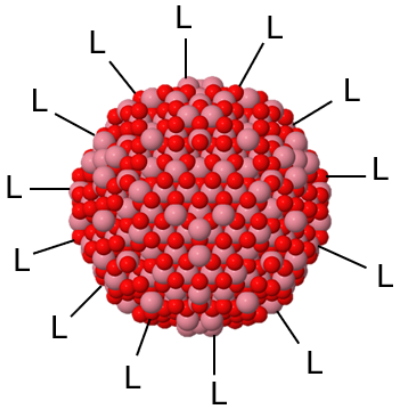
Selected examples

Bimetallic Ru-Co NPs for electrocatalytic HER



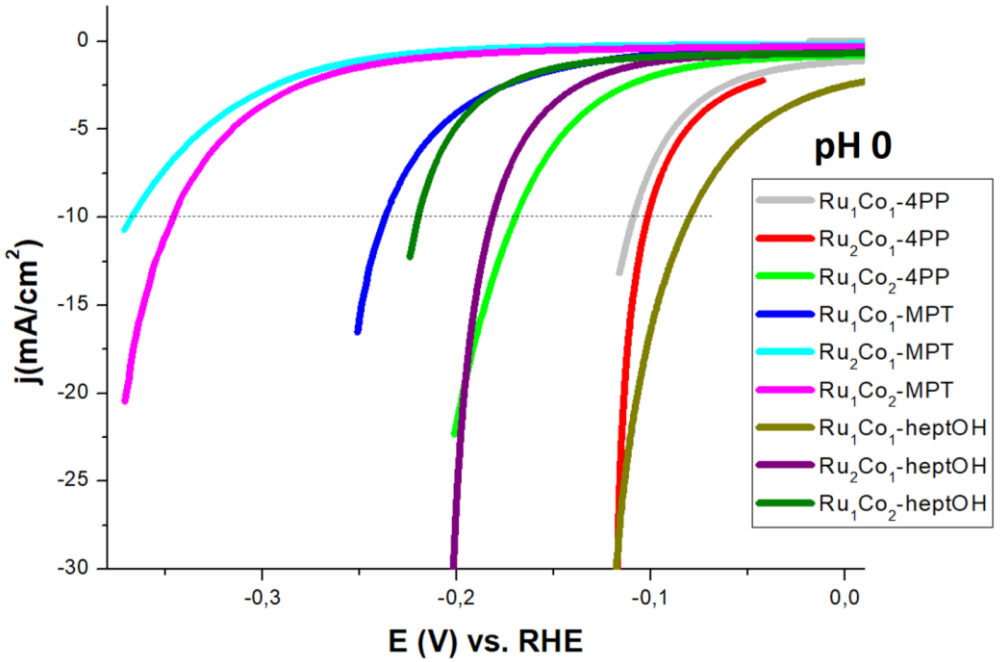


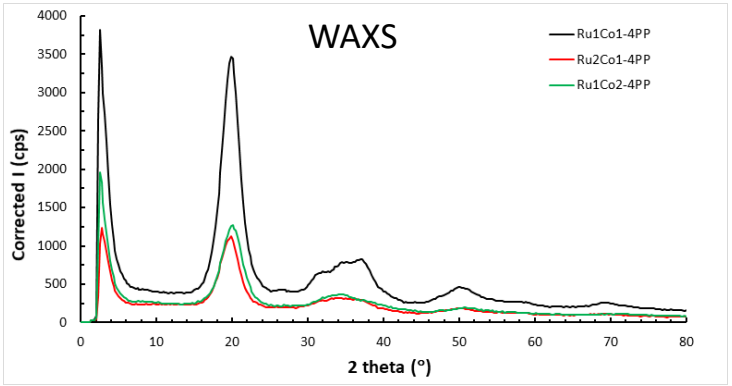
4-PP **MPT** **heptOH**



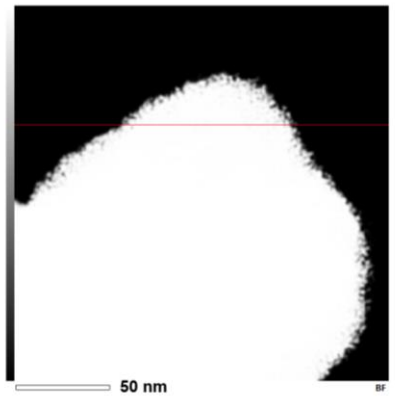
Ru_1Co_1-L, Ru_2Co_1-L, Ru_1Co_2-L

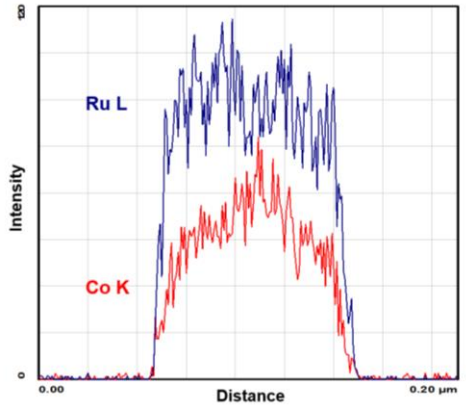
L = 4-PP, MPT, heptOH





In collab. with **Dr. Karine Philippot** (LCC-UPS Toulouse)

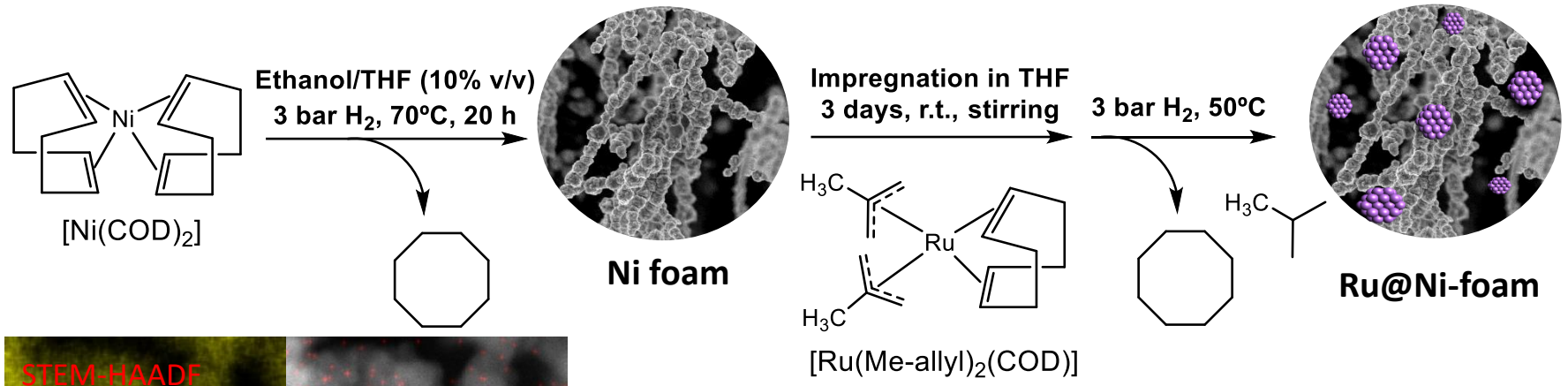




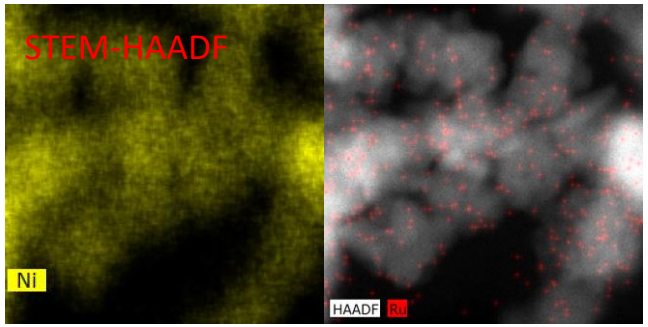
STEM-HAADF image of Ru_1Co_1-4PP

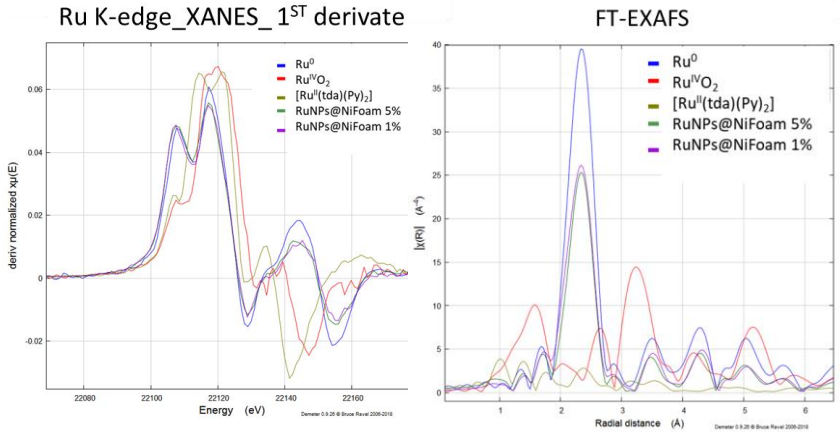
Selected examples

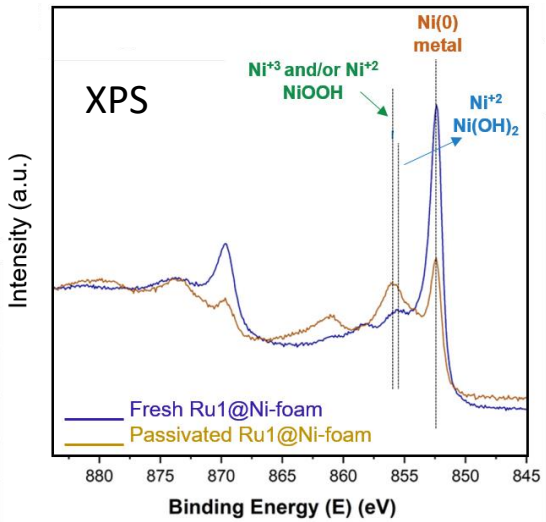
Ru NPs deposited on Ni foam for electrocatalytic HER

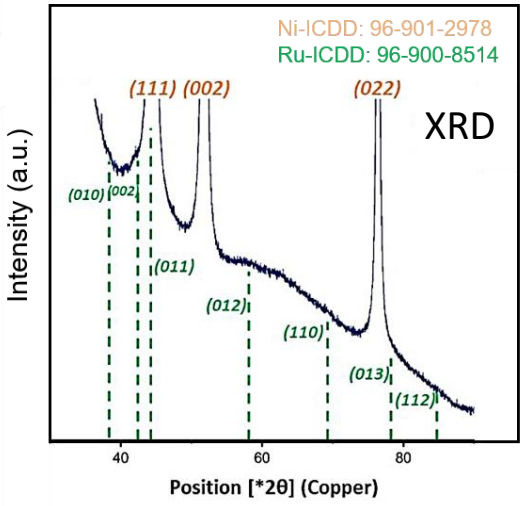


In collab. with **Dr. Nicolas A. Rivas** and **Dr. Alba Garzón** (Max-Planck-Institut Düsseldorf), **Dr. Marcos Gil** (Max-Planck-Institut Mülheim) and **Dr. Karine Philippot** (LCC-UPS Toulouse)

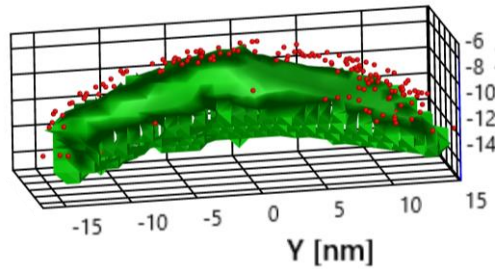








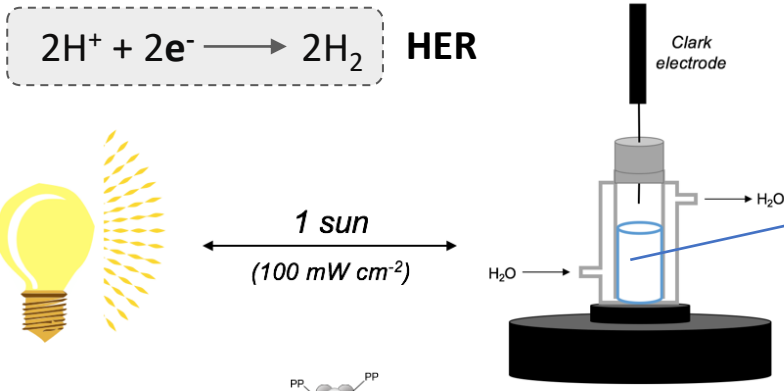
APT

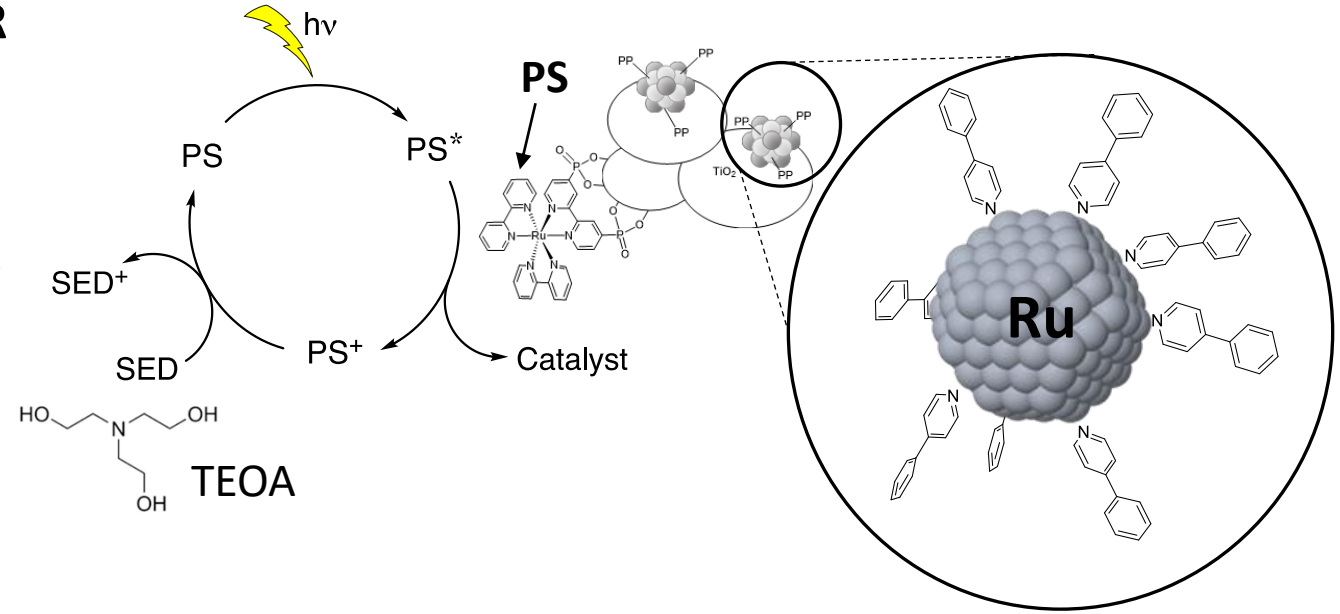


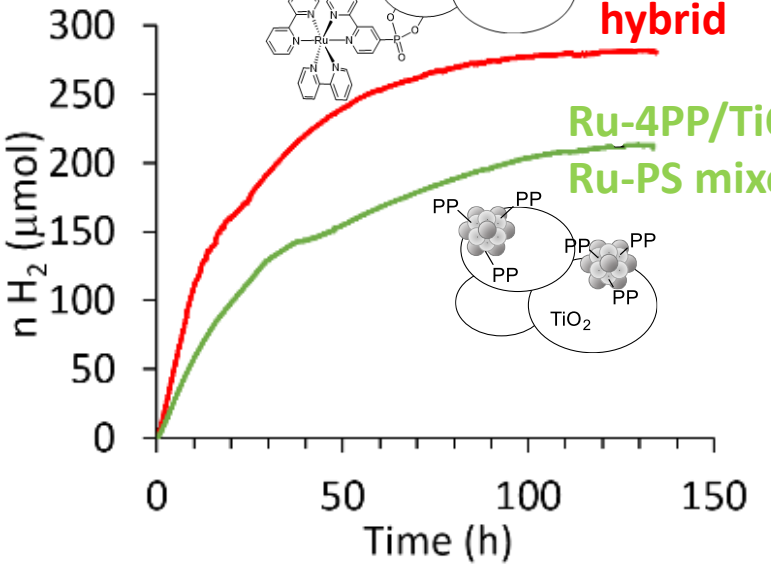
Ru is probably located at the Ni surface as atoms (**SAC** sites)

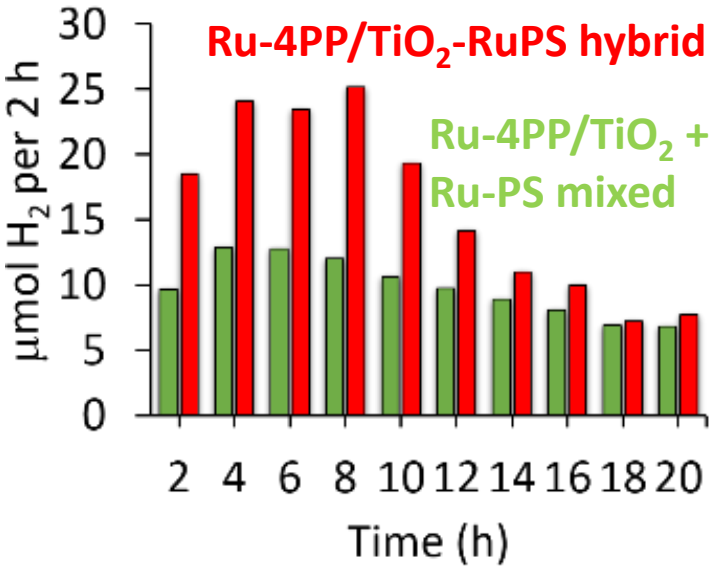
Selected examples

Ru-4PP NPs/TiO_2-RuPS hybrids for photocatalytic HER









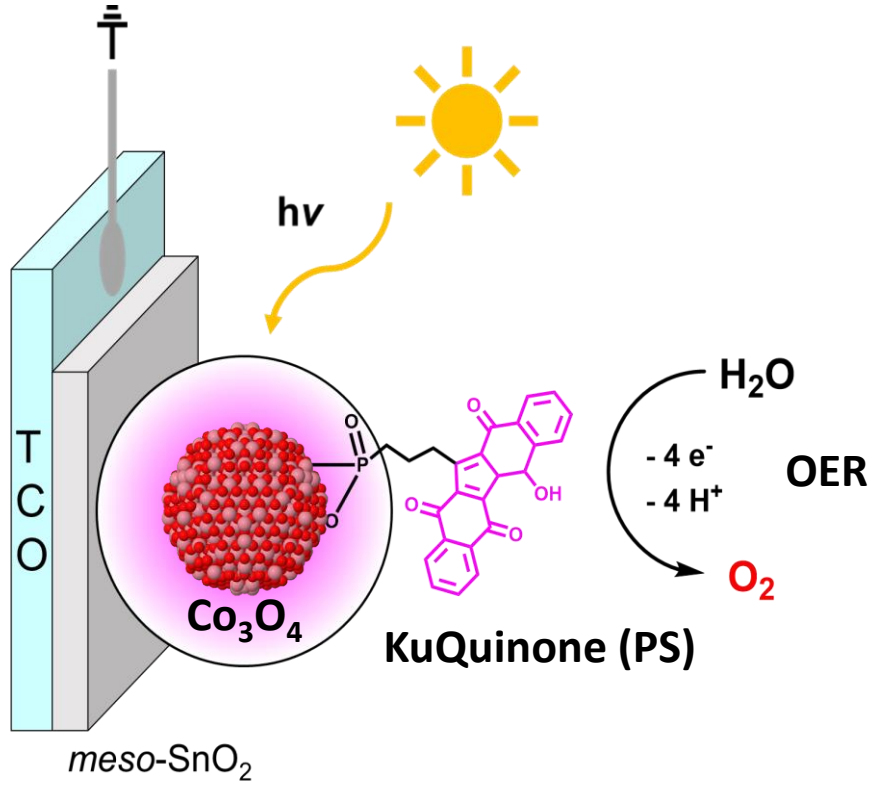
Double role of TiO_2 as a support and electron-mediator

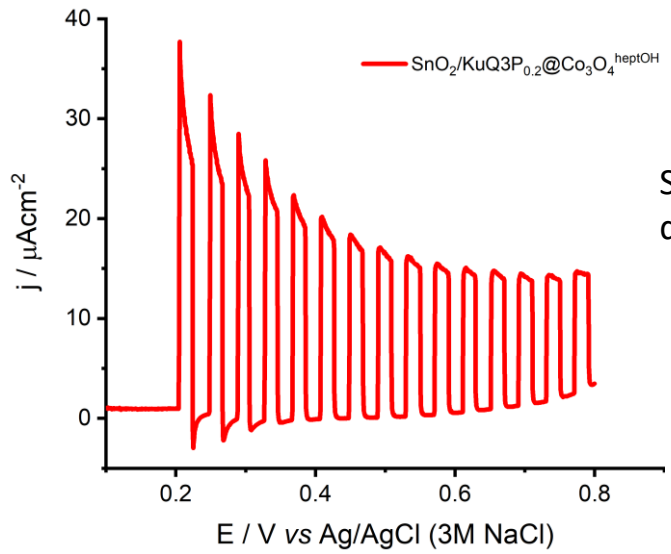
In collab. with **Dr. Mirco Natali** (Univ. Ferrara) and **Dr. Karine Philippot** (LCC-UPS Toulouse)

Sust. Energy & Fuels **2020**, 4, 4170

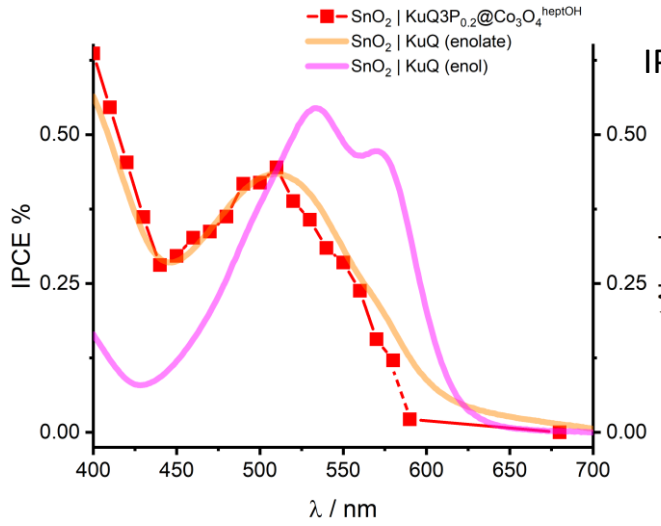
Selected examples

KuQuinones – Co_3O_4 NPs hydrid dyads for photocatalytic OER





Steady-state photocurrent densities of 10 μAcm^{-2}

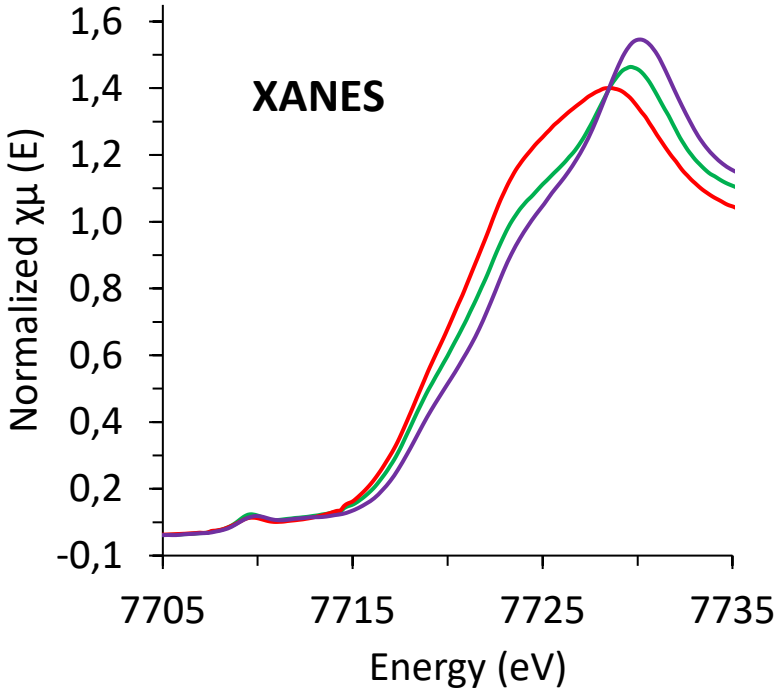


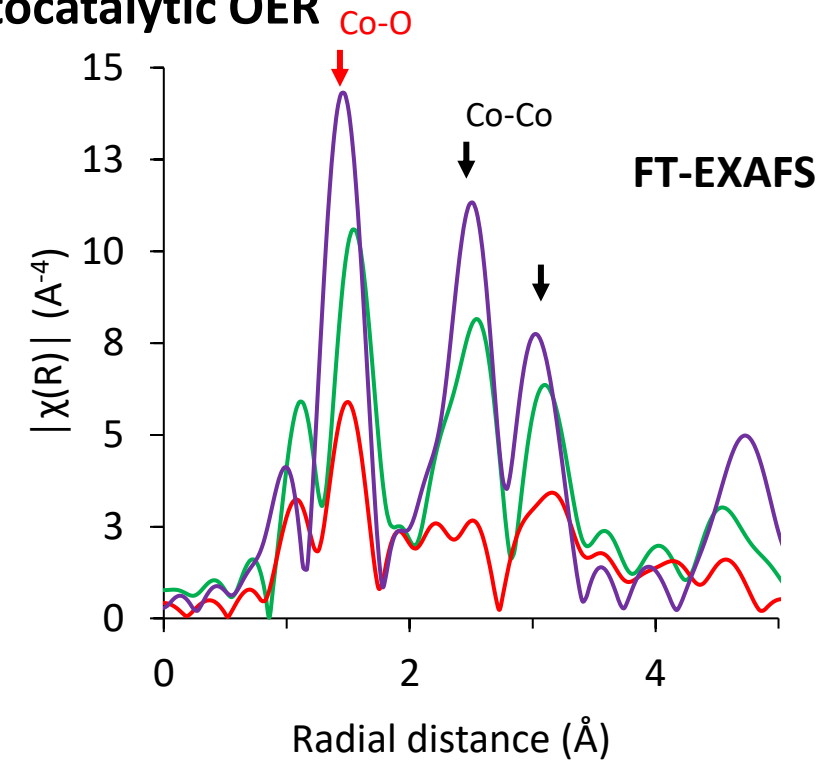
IPCE 0.44% @ 510 nm

In collab. with Dr. **Pierluca Galloni** (Rome, Tor Vergata), **Dr. Mirco Natali** (Univ. Ferrara), **Dr. Andrea Sartorel** (Univ. Padova) and **Dr. Karine Philippot** (LCC-UPS Toulouse)

Selected examples

KuQuinones – Co_3O_4 NPs hydrid dyads for photocatalytic OER





XANES + EXAFS after catalysis: **recovered Co-Co distance** but slightly different spectra, suggesting mixtures of Co_3O_4 and CoOOH

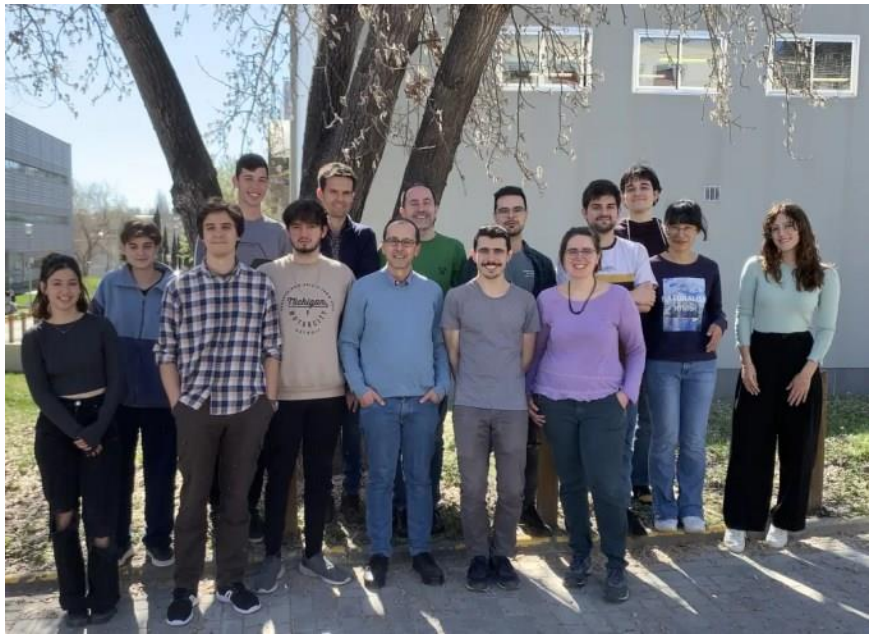
CoOx as catalytic active species after fast decomposition of "Co-atoms" (SACs) under irradiation

In collab. with Dr. **Pierluca Galloni** (Rome, Tor Vergata), **Dr. Mirco Natali** (Univ. Ferrara), **Dr. Andrea Sartorel** (Univ. Padova) and **Dr. Karine Philippot** (LCC-UPS Toulouse)

BL22 CLAESS, ALBA Synchrotron

In collab. with **Dr. Marcos Gil-Sepulcre** and **Dr. Serena DeBeer** (Max-Planck-Institut Mülheim)

Selective RedOxCatalysis (SelOxCat) Group - UAB



Many thanks for your attention

SelOxCat
Selective RedOx Catalysis