



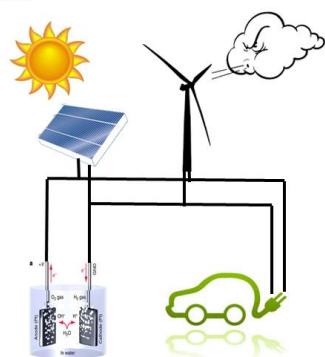
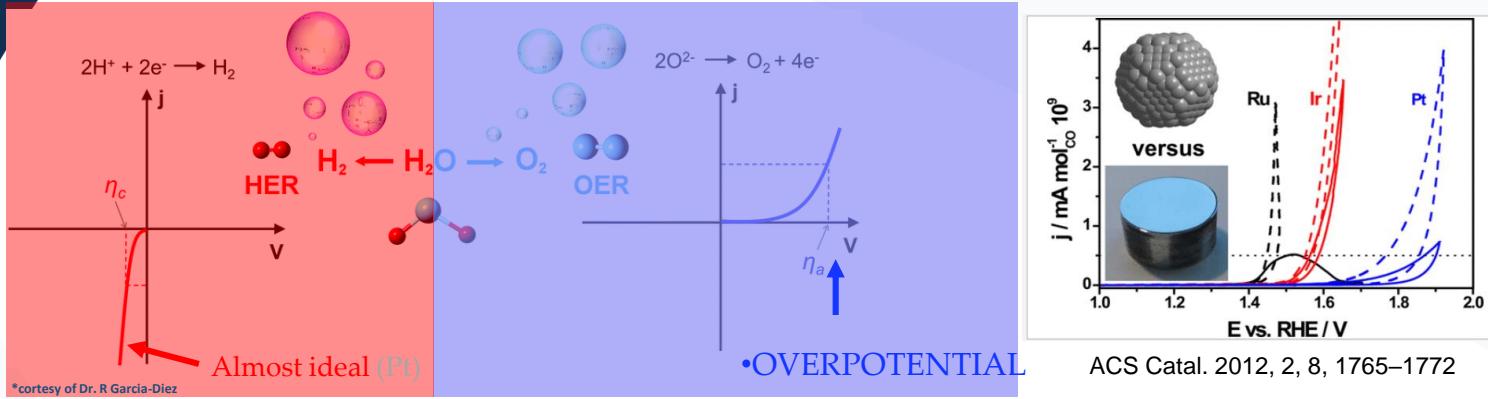
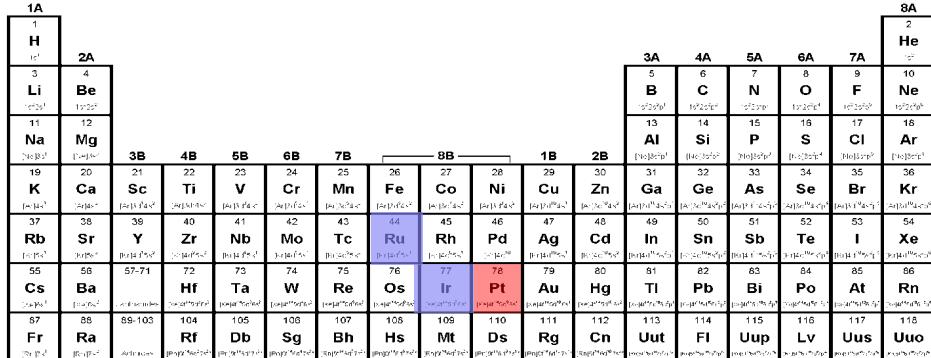
TR Plan de Recuperación,
Transformación
y Resiliencia



Controlling the number of coordinatively unsaturated iridium oxide active centers for optimize the electrocatalytic oxygen evolution reaction

Juan J. Velasco Vélez
2nd September

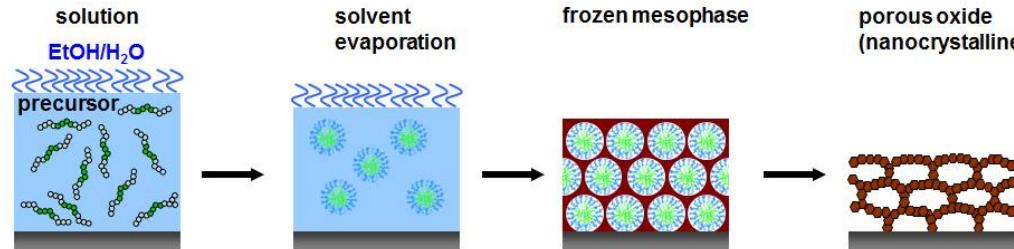
Oxygen evolution reaction (OER)

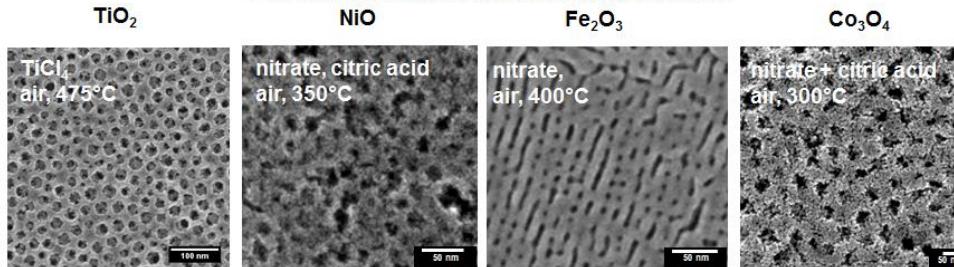
A periodic table highlighting transition metals (Groups 3B to 7B) in purple, which are key catalysts for the Oxygen Evolution Reaction (OER).

Mesoporous electrodes

Porous templated oxide films via EISA (Evaporation induced self assembly)



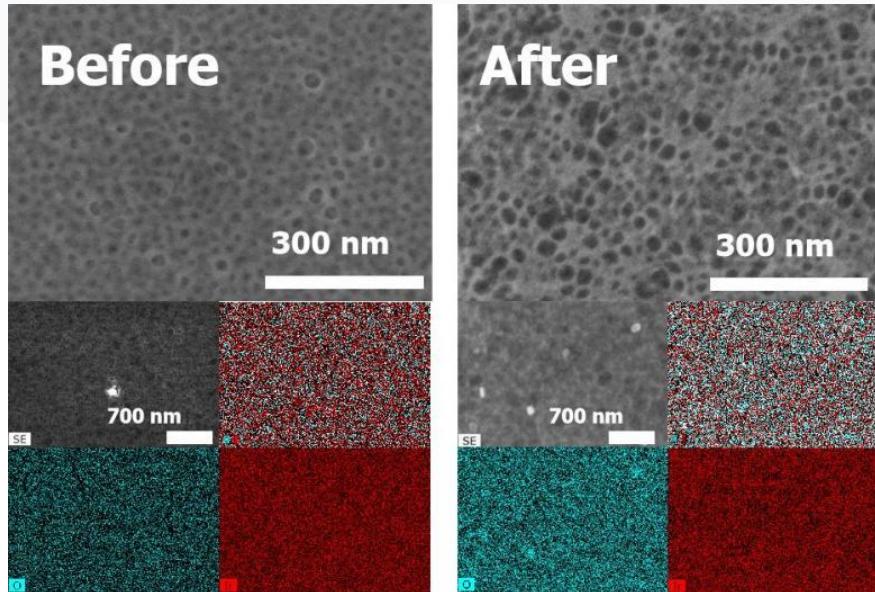
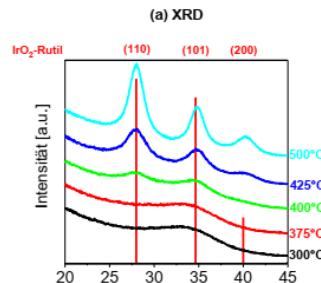
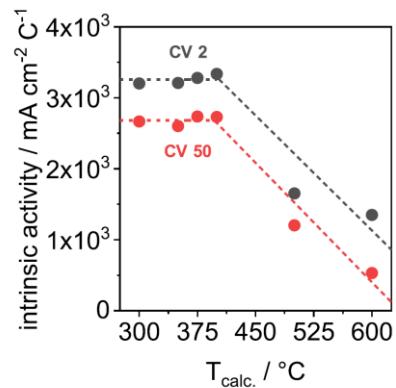
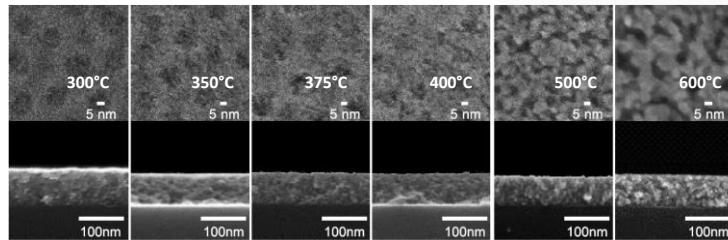
Different metal oxides accessible



The mesoporous IrO_x film was prepared by iridium acetate and micelles of amphiphilic block-copolymers using an evaporation-induced self-assembly (EISA) method, where the pore size is accurately controlled by the triblock copolymer.

Chemistry of materials 2013, 25(14), 2749-2758.

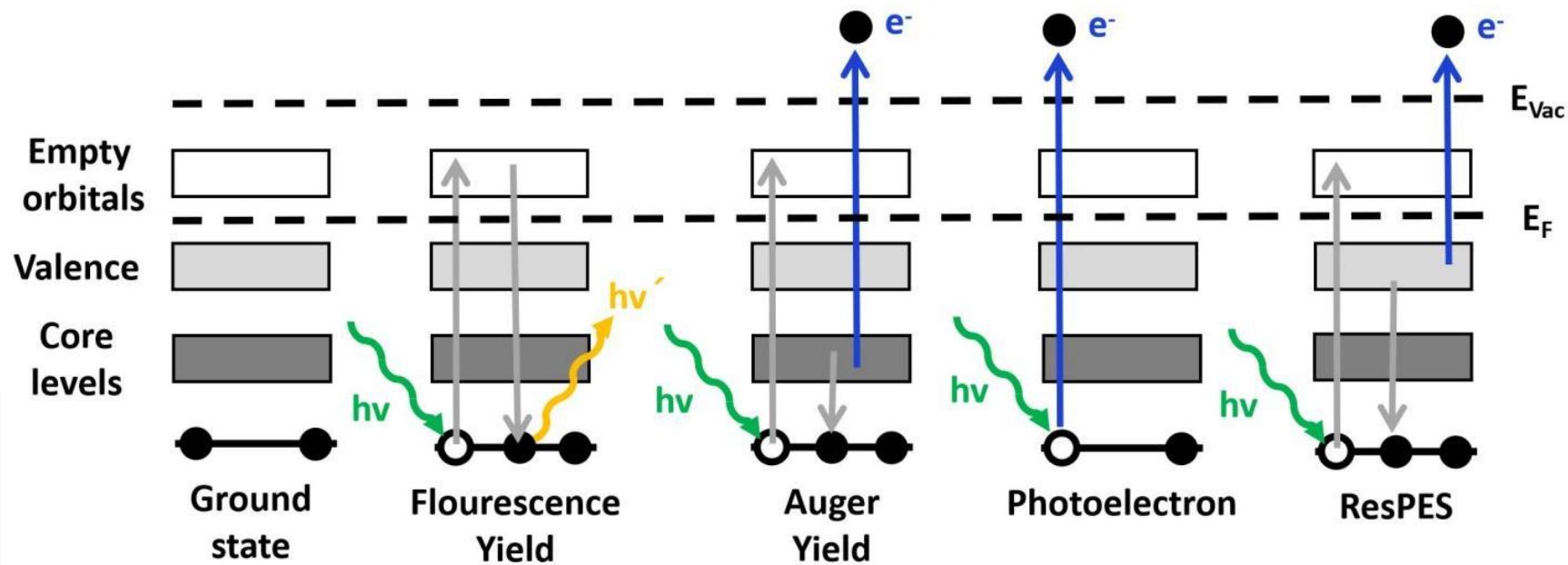
Mesoporous electrodes



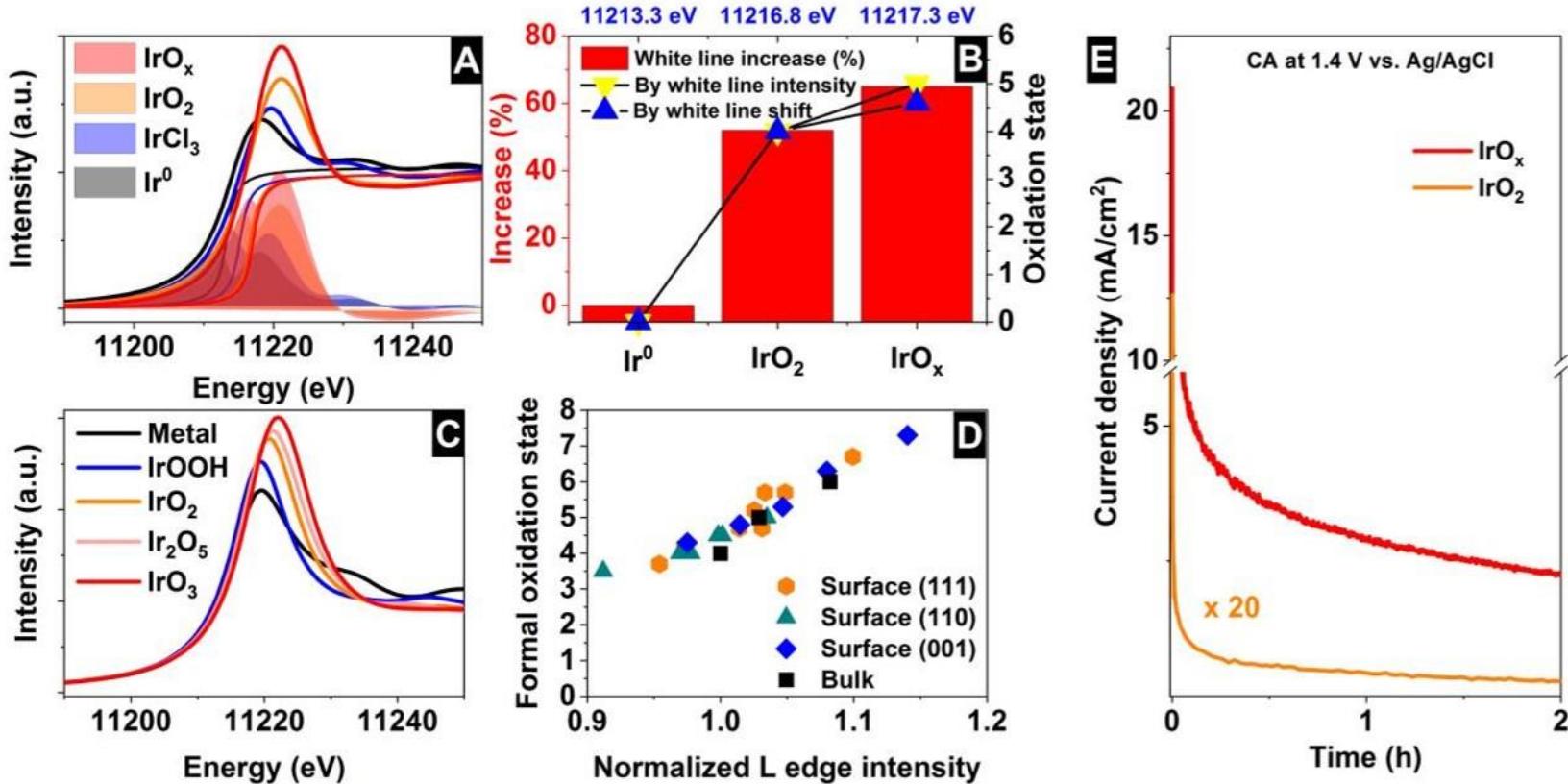
Journal of The Electrochemical Society 2016, 163(11), F3132: **For calcined iridium films the optimal balance between activity and stability is reached between 400°C and 500°C.**

Chemistry of materials 2013, 25(14), 2749-2758.

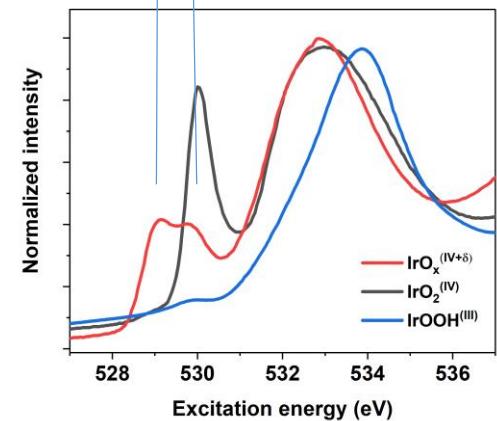
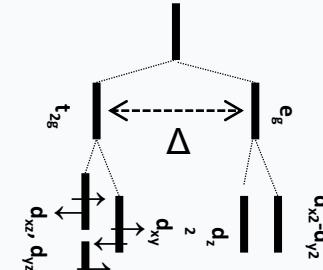
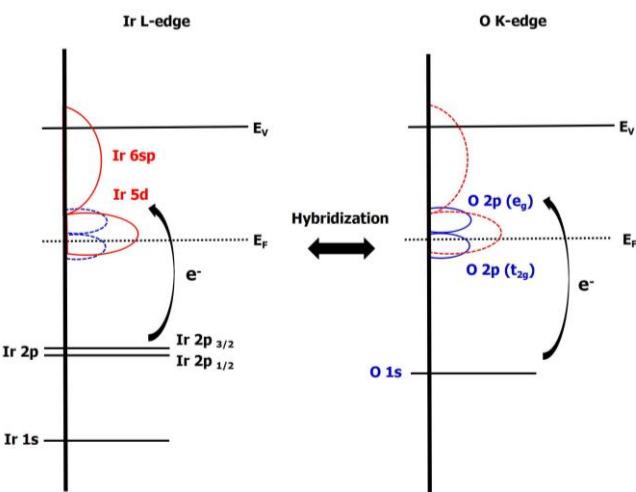
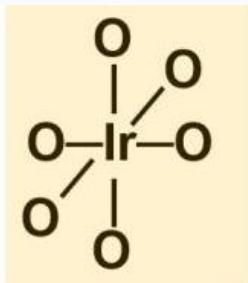
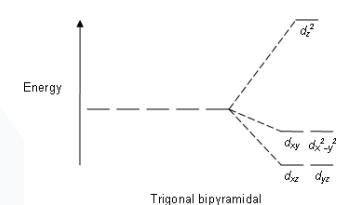
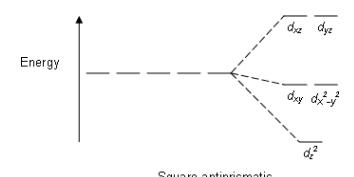
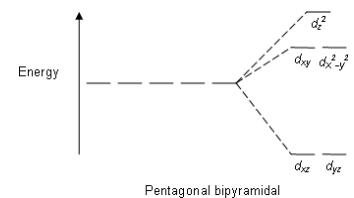
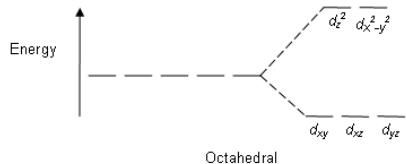
Photoelectron spectroscopy

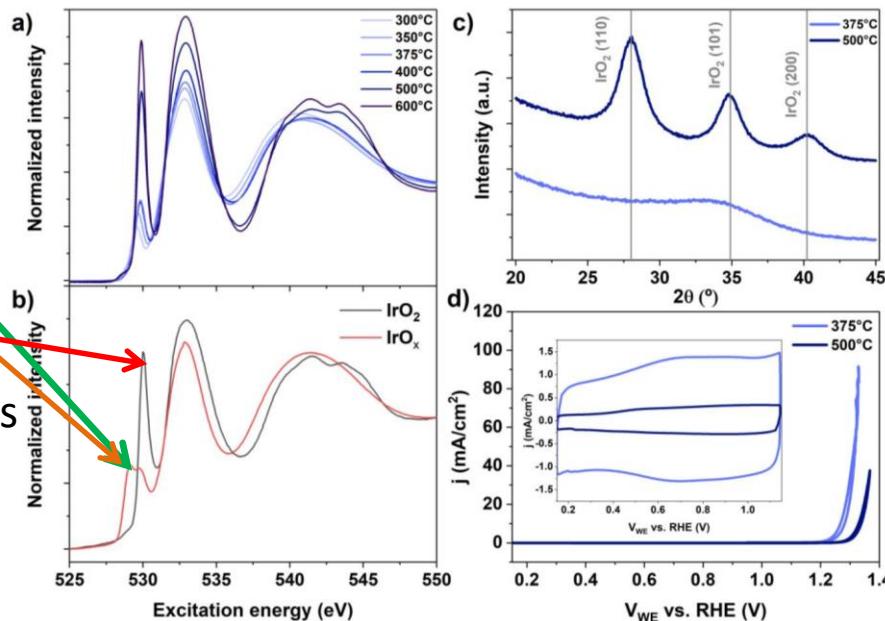
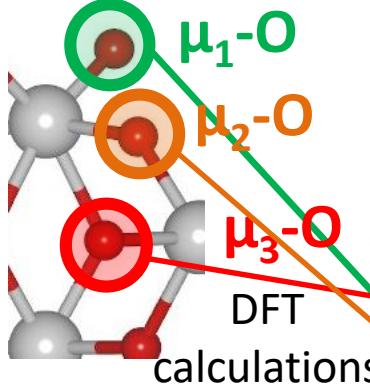
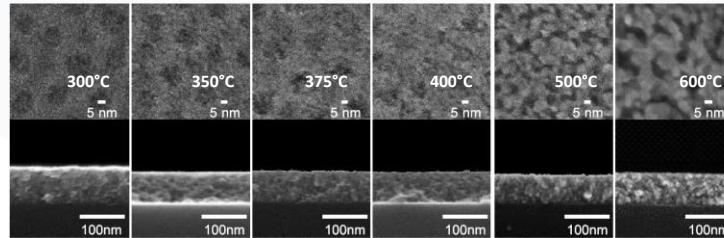


Ex situ, references samples

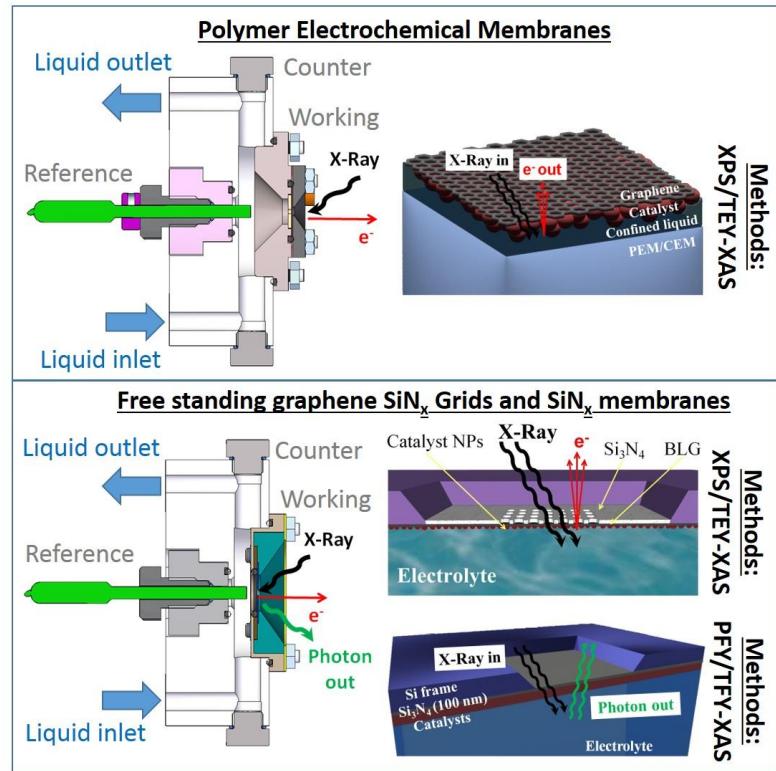
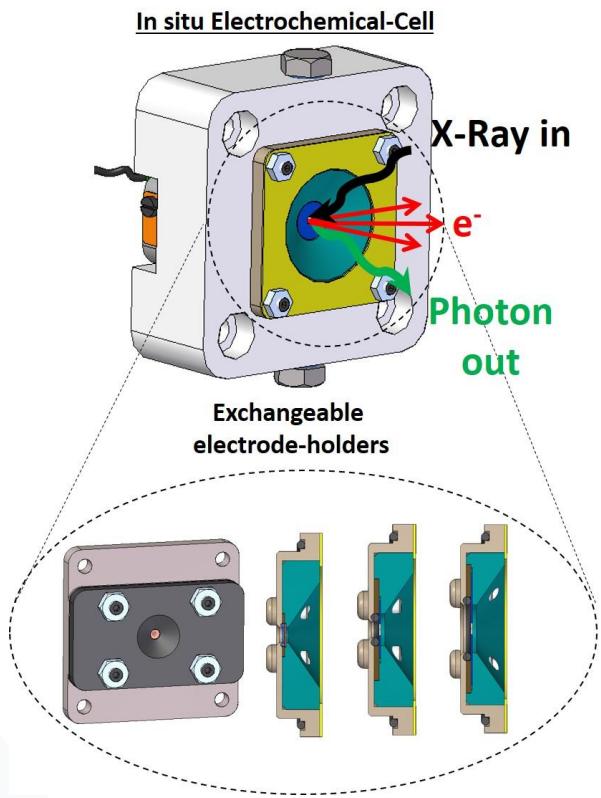


Oxidation state (crystal field) IrO_x

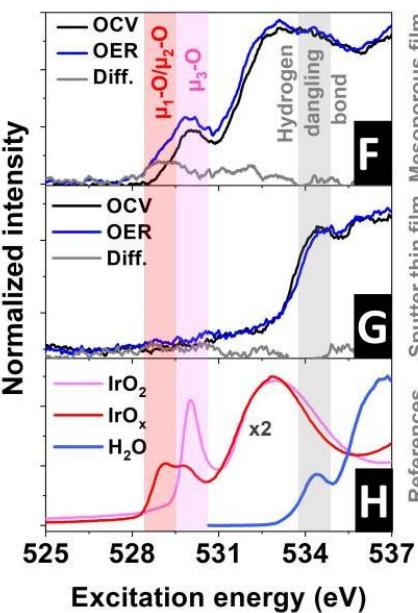
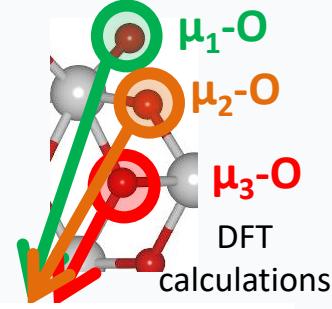
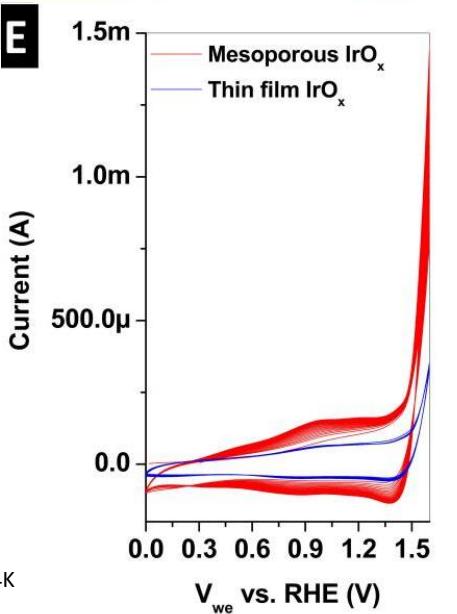
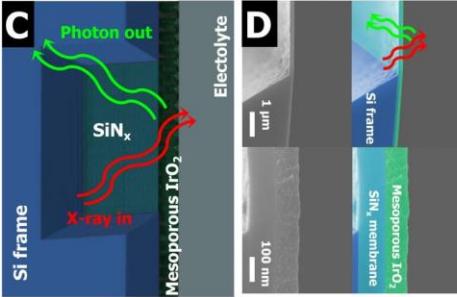
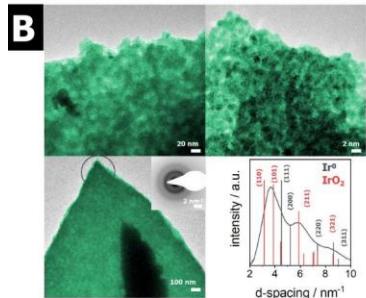
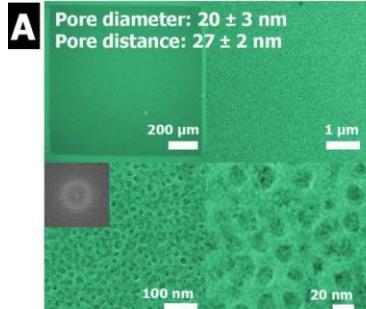




Operando electrochemical cell



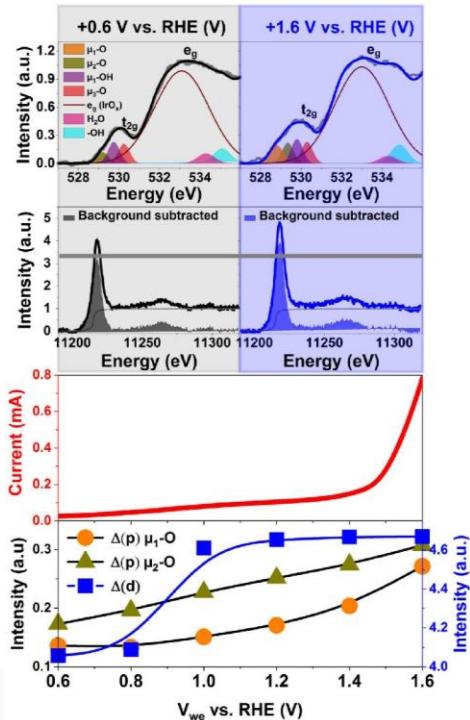
OER on IrO_x (Photon-in/Photon-out)



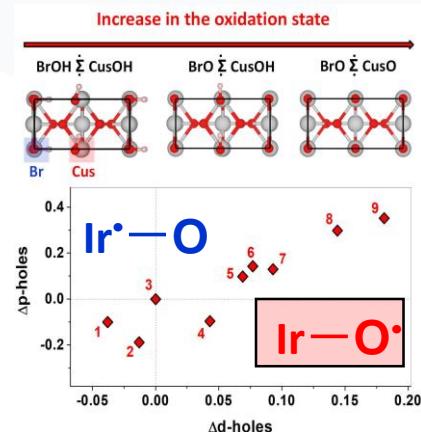
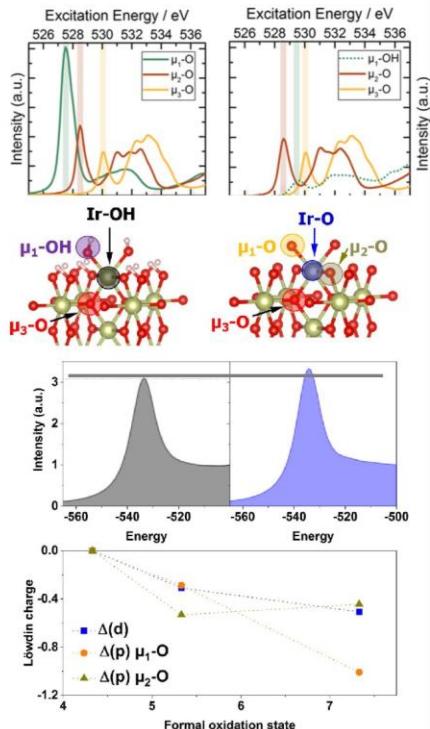
Dr. D. Bernsmeier (TU Berlin)

In situ O K-edge + Ir L₃-edge

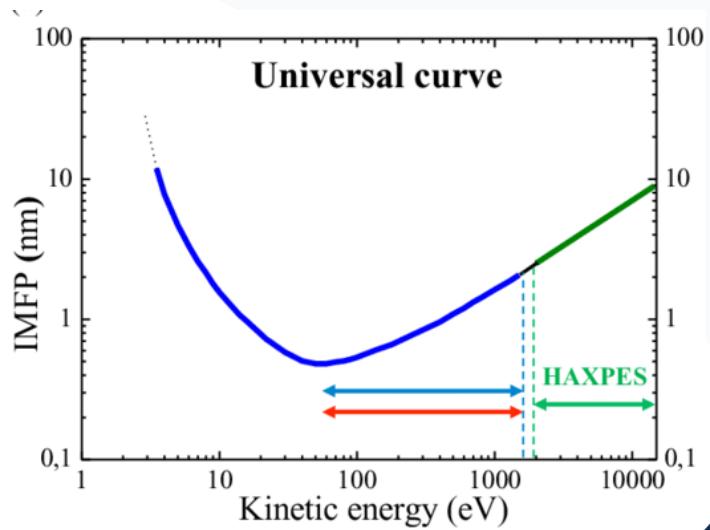
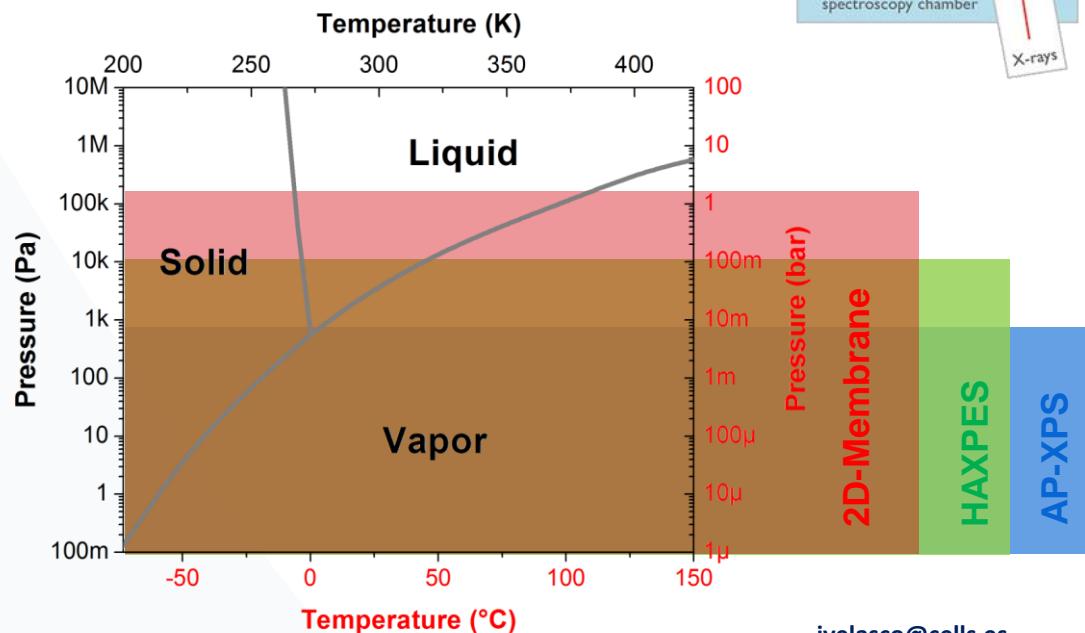
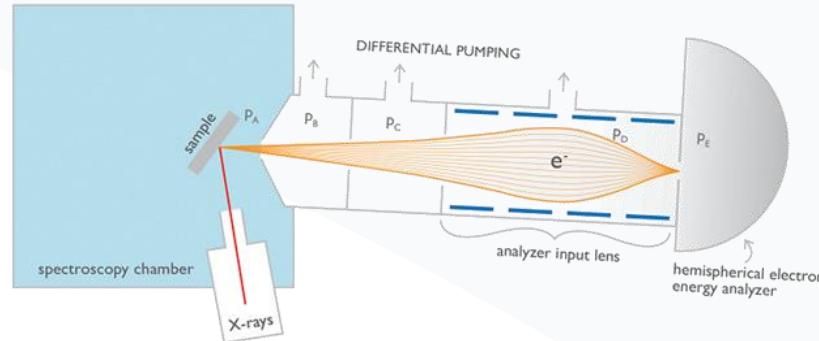
Measurements



Calculations



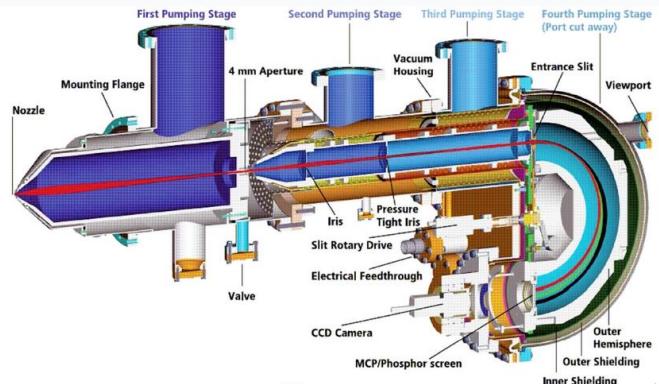
NAP-XPS



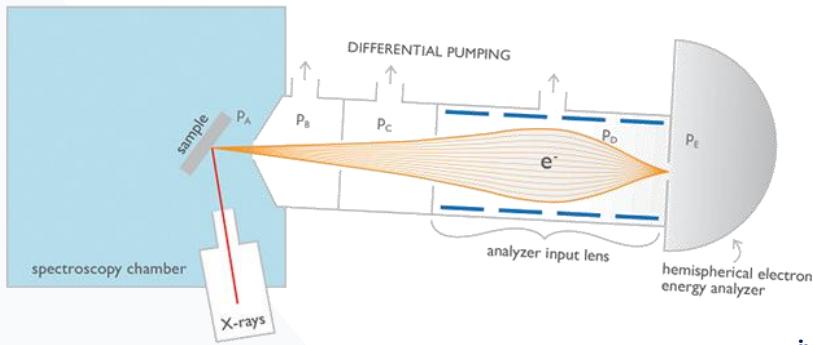
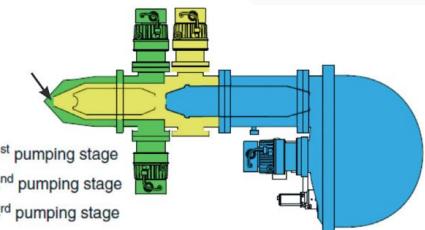
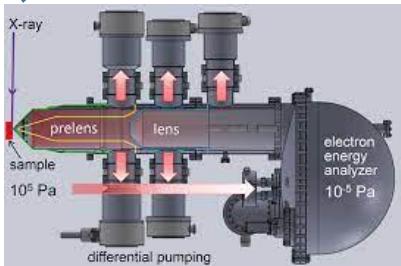
NAP-XPS

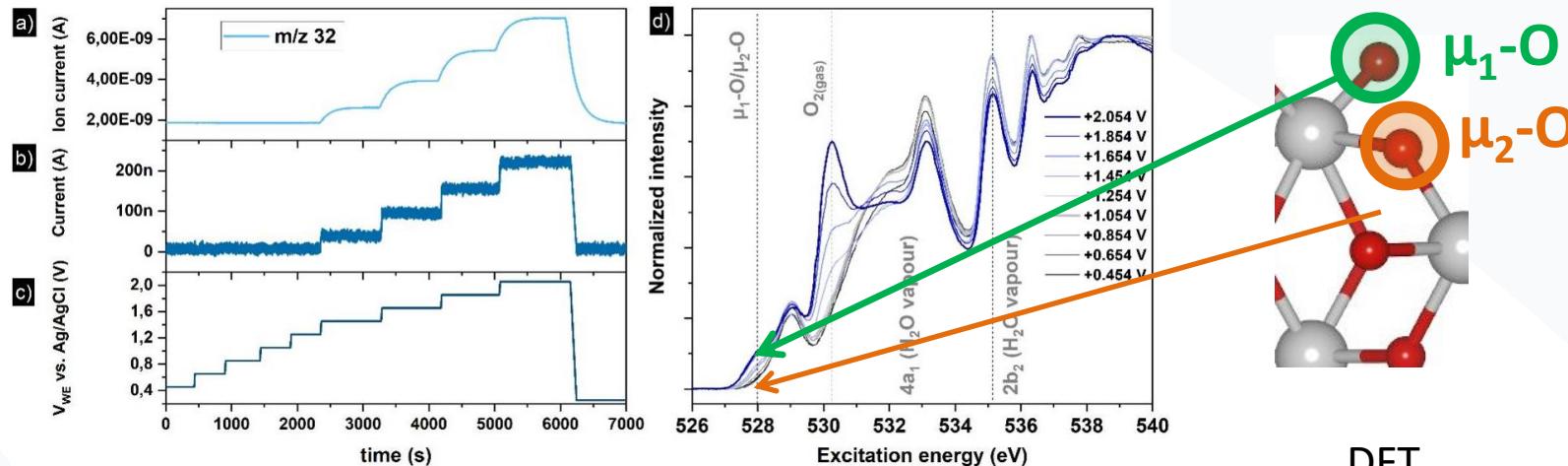
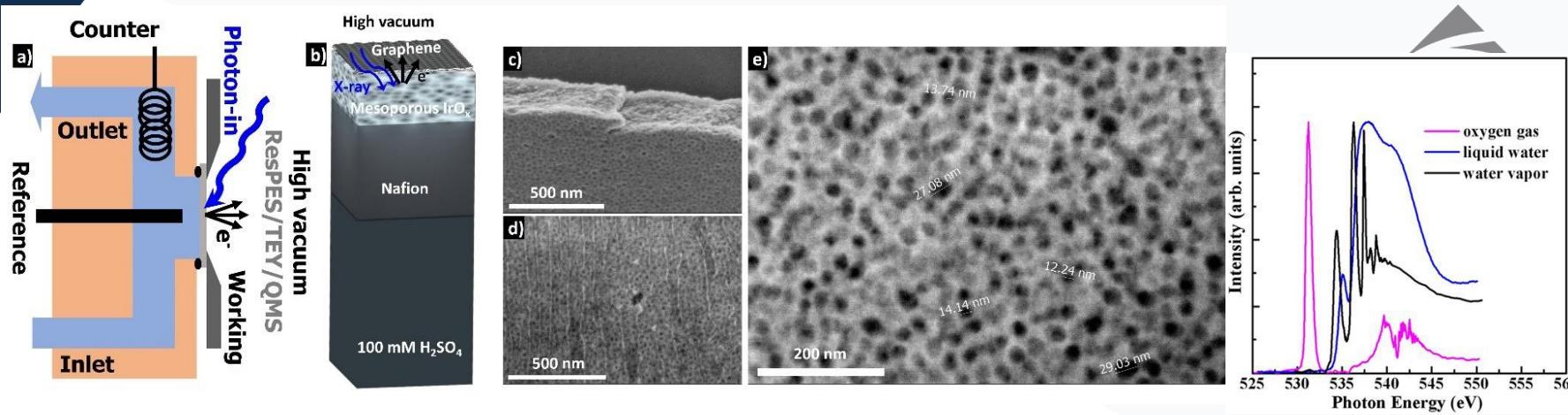


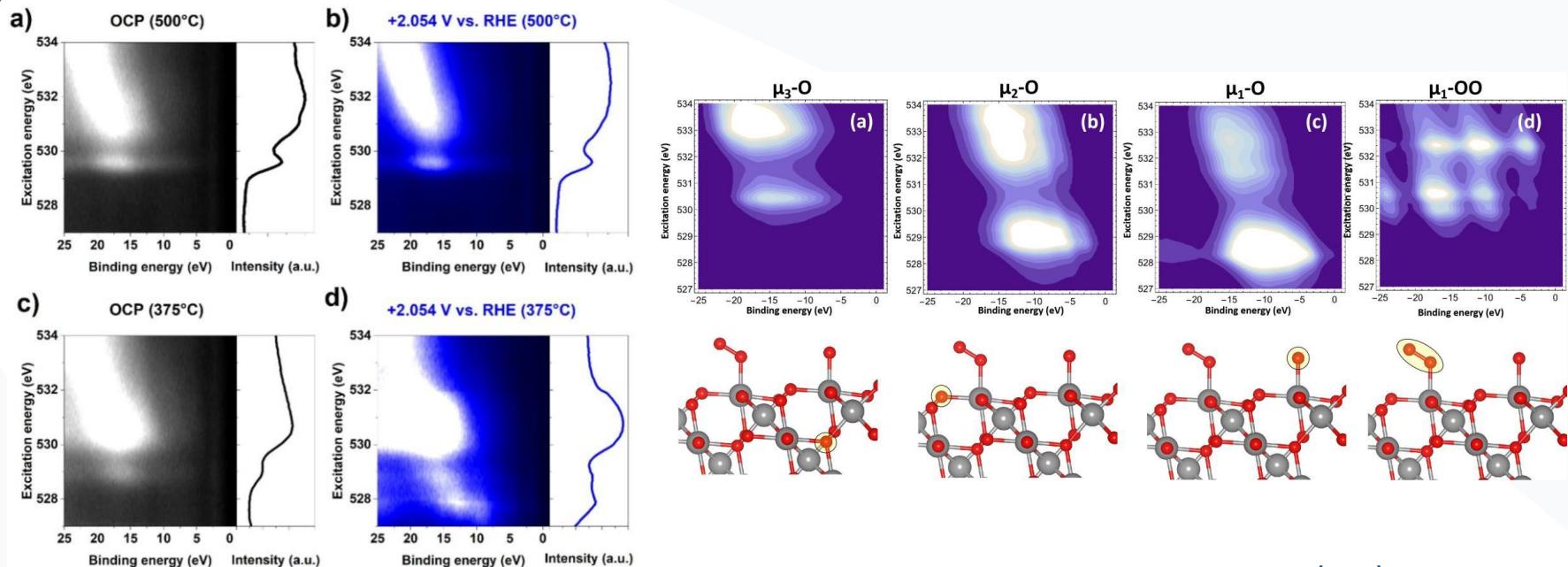
PHOIBOS 150 NAP analyzer



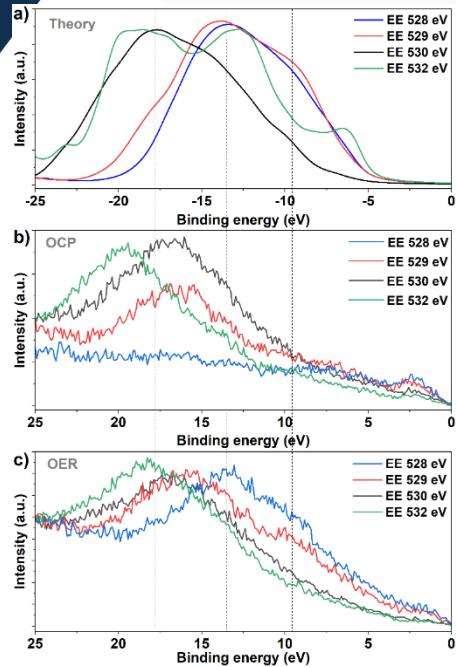
HiPP-3 NAP analyzer



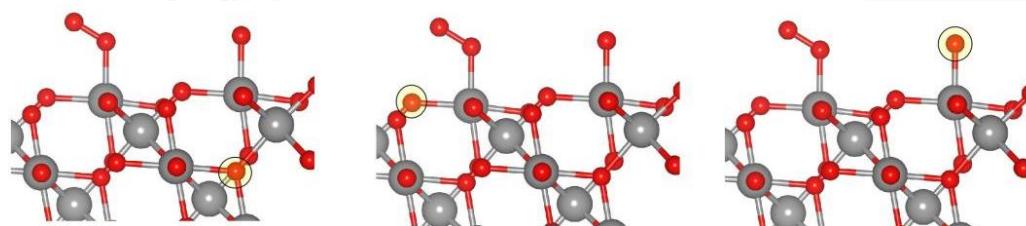
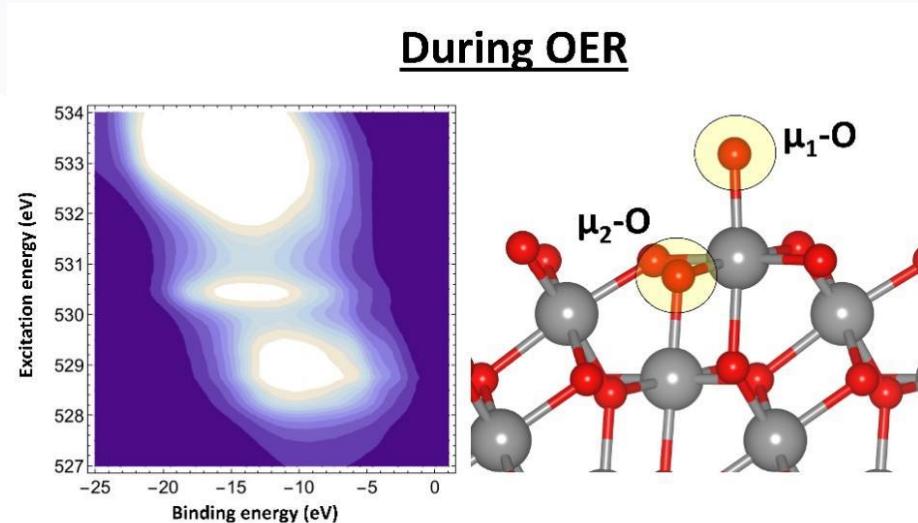




Advanced Energy Materials (In press) DOI: 10.1002/aenm.202303407



a) Calculated resonant Auger spectra of oxygen species on the (110) and (111) surfaces of rutile-type IrO_2 . The computed EE of the various species are ca. 530 eV for the $\mu_3\text{-O}$ and $\mu_2\text{-OH}$, 529 eV for the $\mu_2\text{-O}$ and $\mu_1\text{-OH}$, 528 eV for the $\mu_1\text{-O}$, and 532 eV for the $\mu_1\text{-OOH}$ and $\mu_1\text{-OO}$. Measured spectra under b) OCP and c) OER conditions.



$\mu_3\text{-O}$ (stability)

$\mu_2\text{-O}$ (Surface electron hole)

$\mu_1\text{-O}$ (Surface active species)

New beamline in ALBA synchrotron

3SBar will combine ambient pressure X-ray Photoemission Spectroscopy (AP-XPS) at high pressures (1 bar or more) and surface X-ray diffraction (SXRD) at grazing incidence angles. First beamline optimized for ALBA II.

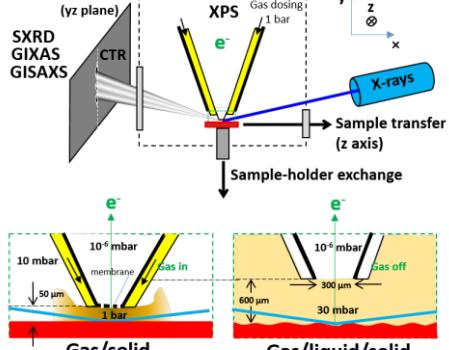
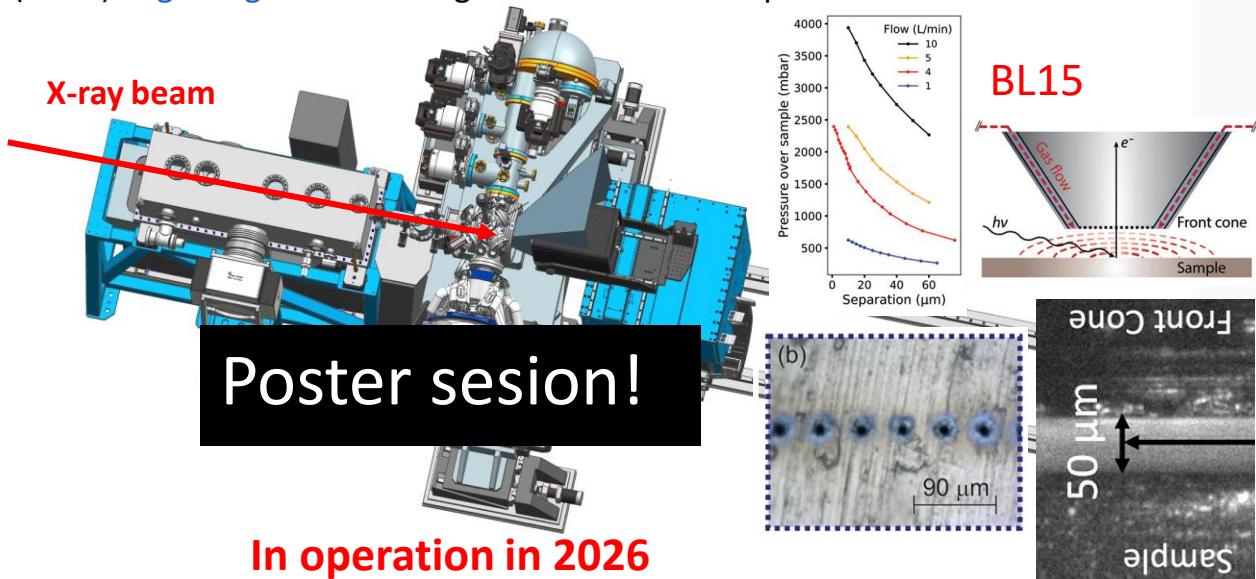
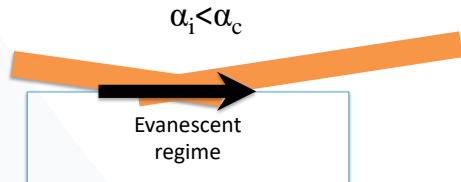


Fig. 1: a) Top-view description of the 3Sbar approach (see also Figs. 15-17). b) schematic zoom-in description of the sample/analyzer front-cone geometry for gas/solid and gas/liquid/solid experiments.



In operation in 2026

Surface sensitivity
Total external reflection: X-ray depth control
Signal enhancement!

Acknowledgments



T. Jones

Denis Bernsmeier

P. Zeller

R. Mom

Yang Shao-Horn

A. Knop-Gericke

B. Roldan Cuenya

Robert Schlögl

3Sbar team

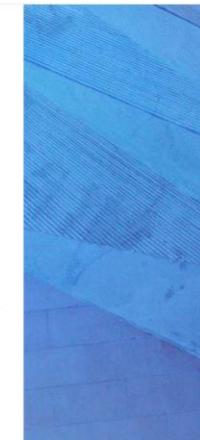


BL Scientist 3sBAR within the framework of
the Recovery, Transformation and Resilience
Plan

Reference 2023-256-2

Deadline 16/09/2024

Division Experiments



<https://public.cells.es/jobs/#!/jobs/bl-scientist-3sbar-within-the-framework-of-the-recovery-transformation-and-resilience-plan>