Collaboration projects with ALBA

The process for the selection of the projects to be awarded a post-doc position within the FCT-ALBA collaboration agreement is now finished. The abstracts of the selected projects as well as its teams and scientific areas are published at continuation.

Scientific area 1: Multi-length scale imaging in life sciences.

Imaging phosphorylation-dependent stress response pathways in prokaryotic and eukaryotic cells

Célia Romão (ITQB, Portugal), Federico Herrera (U Lisboa, Portugal), Vanesa Martin (U Oviedo, Spain), Eva Pereiro (BM09-MISTRAL, ALBA, Spain) and Roeland Boer (BL13-XALOC, ALBA, Spain)

The present proposal aims to unveil the potential role of specific phosphorylation events in the stress responses of prokaryotic and eukaryotic cells. The DNA-binding proteins Dps1 and Dps2 are involved in metal storage and DNA protection in the bacterium *Deinococcus radiodurans*, being key players in its extreme resistance to stress. Our preliminary results indicate that their function is dependent on their phosphorylation and the intracellular distribution of metals, such as calcium. Signal Transducer and Activator of Transcription 3 (STAT3) is a pleiotropic transcription factor that regulates eukaryotic cell proliferation and differentiation, apoptosis, inflammation and response to diverse types of stress. STAT3 is constitutively activated by phosphorylation in 70% of solid tumors, including glioblastoma, where it is essential for cancer cell survival and proliferation. We have recently described that asymmetric post-translational modifications produce striking changes in the intracellular distribution of STAT3 dimers, leading them to mitochondria and possibly to mitochondrial-associated membranes (MAMs). We will take a multidisciplinary approach using correlative microscopy and cryo soft X-ray tomography, as well as X-ray structural studies, to establish with an unprecedented precision the dynamics of Dps proteins and STAT3 dimers upon exposure of *Deinococcus radiodurans* and glioblastoma cells to stress/inflammatory cues.

Scientific area 2: Rational design of catalysts.

Data analysis-guided multimodal spectroscopy to unveil atomic dynamics in nanosized metal aggregates under methane decomposition

Adélio Mendes (U Porto, Portugal), Patricia Concepción (ITQ, UPV-CSIC, Spain), Klaus Attenkofer (ALBA, Spain)

Catalytic methane decomposition is a promising technology producing COx free hydrogen and solid carbon, providing decarbonized energy at the same time it removes CO2 from the atmosphere at competitive cost. However, catalyst deactivation by carbon coverage has hindered industrial application, being fundamental understanding of the reaction process needed for a rational design of more active, stable and regenerable solid catalysts. The objective of the project is to achieve an atomic-level understanding of the dynamics between surface and subsurface carbon species coming from methane decomposition and the catalytic metal nanocrystals, which determine activity and longterm stability of the catalysts. This information will be retrieved at the facilities of the ALBA Synchrotron Light Source facility, which combined with data analytic and with the spectroscopic studies performed at ITQ will set the bases for a rational design of advanced solid catalysts with technologically significant performance in

H2 generation targeting a very fast energy decarbonisation economy. This new coordinated project will allow consolidating the interaction between the research groups and increase competitiveness by optimizing resources and infrastructure of the different groups.

Scientific area 3: Electrical storage: E-mobility in an economic and environmental context.

Rational design of advanced electrode materials based on synchrotron X-ray characterization for next generation high-performance lithium batteries

Lifeng Liu (INL, Portugal), Dino Tonti (ICMAB-CSIC, Spain), Laura Simonelli (ALBA, Spain)

Rechargeable lithium (Li) batteries are a key enabler to decarbonizing EU's transport and energy sectors, thereby contributing to reaching the climate neutrality by 2050. The European Battery Alliance estimates that the battery market will be 250 € billion from 2025 onwards, which is strategically important to Europe. To advance rechargeable Li battery technologies and accelerate their widespread deployment, there is a pressing need for research, development and innovation (R&D&I) on advanced electrode materials and cell chemistries to address major challenges for improving batteries performance. In this project, the International Iberian Nanotechnology Laboratory (INL) will join forces with ALBA Synchrotron and the Institute of Materials Science of Barcelona (ICMAB-CSIC), taking advantage of the state-of-the-art ex-situ and *operando* synchrotron X-ray characterization capabilities available at ALBA, to work towards comprehensive and in-depth understanding about the evolution of crystal phases, atomic structures, morphology, local coordination chemistry, lattice strain and electronic structure of various electrode materials upon battery charge and discharge. The fundamental insights gained will be used to guide the design and synthesis of cost-effective silicon anodes for advanced Li-ion and solid state Li batteries, and Li metal/alloy anodes as well as catalytic cathodes for Li-sulfur and Li-air batteries. The project will reinforce ALBA's material analysis capabilities and its competences in battery research, promote the collaboration between Portuguese and Spanish research institutions on this strategically important area, and consolidate Iberia's effort towards the R&D&I activities on batteries.

Scientific area 4: Electronic structure of new materials

Emergent magnetic and electronic properties of novel 2D layers and Moiré structures of Van-der-Waals Quantum Materials (2DMoireMagQMs)

Joaquin Rossier (INL, Portugal), Sergio O. Valenzuela (ICN2, Spain), Efrén Navarro (ICMOL, U. Valencia), Manuel Valvidares (BL29-BOREAS, ALBA, Spain)

We propose to develop novel 2D layers and "moiré" structures of magnetic Quantum Materials of Van-der-Waals type not realized or explored to date, in order to produce and investigate emergent electronic and magnetic states arising by the rupture of crystal symmetry and the frustration of electronic and magnetic orders characteristic of bulk forms. For fabrication, we will combine top-down (cleaving, exfoliation) and bottom-up (evaporation, epitaxy) approaches with deterministic transfer in inert atmosphere (glove boxes) and/or clean room environments. The structural, electronic and magnetic properties of the systems will be investigated by complementary synchrotron radiation (ALBA), high-resolution transmission electron microscopy (INL and BIST) and laboratory techniques (ICN2, Univ. Valencia). More specifically, magnetic properties will be characterized using magneto-optical Kerr effect (MOKE) and x-ray magnetic circular dichroism (XMCD), with spatially resolved information provided via x-ray microscopy; transport properties will be investigated by sheet resistance and Hall-type of measurements; electronic structure will be revealed via angle-resolved photo-emission spectroscopy (ARPES), while structural properties will be characterized by high resolution electron microscopy (SAED, Lorentz, EELS), x-ray diffraction and Raman-Photo-luminescence spectro-microscopy. The most relevant systems and results will be supported by theory calculations at INL.