ALBA II Symposium

Report of Contributions

https://indico.cells.es/e/ALBA_II

Contribution ID: **1** Type: **not specified**

Introduction and Background

Thursday, 18 January 2024 14:30 (15 minutes)

Session Classification: Introduction and Background

Contribution ID: **2** Type: **not specified**

Multilength Scale Imaging of Cement Hydration

Thursday, 18 January 2024 15:15 (30 minutes)

Portland cements are environmentally contentious, accounting for ≈7% of anthropogenic CO2 emissions. If cement production is considered a country, it would be the third emitter just after China and USA. Hence, developing concretes with lower embodied carbon contents is central to maintaining our well-being. The main drawback of the most ambitious proposals for sustainable low-carbon cements is their slow hydration kinetics in the first three days. This is the focus of many hundreds of researchers and mine.
My original contribution is to develop 4D (3D+time) cement hydration nanoimaging within a multiscale framework with the final aim to decrease the CO2 emissions. Full-field laboratory X-ray micro Computer Tomography (μCT) is widely used to study cement hydration but the best spatial resolution is about 2 μm for a Field of View (FoV) of ≈ 1×2 mm (H×V) with measurements taking hours. Moreover, the contrast between the different components is poor. Full-field propagation-based phase-contrast synchrotron X-ray μCT can study similar FoVs ≈ 1×2 mm with better spatial resolution, close to 0.50 μm. The measurements are fast, i.e. 5-10 minutes. Unfortunately, the contrast is only slightly better and its availability is scarce. Cement hydration can be studied with much better contrast and spatial resolution by scanning near-field ptychographic nano-computed tomography (nCT). In this case the FoV could be of the order of ≈ 200×30 μm with spatial resolution, close to 250 nm, and excellent component contrast. Even air and water can be differentiated. Unfortunately, these nCTs takes about 3-4 hours in optimized beamlines (BL) at third generation synchrotrons. Example of different imaging modalities for 4D nCT and μCT cement hydration will be discussed. Finally, some expected performances at CoDI (ALBA-II optimized BL to be built) will be commented.

Presenter: Prof. GARCÍA ARANDA, Miguel Ángel (Univ. Malaga)

Contribution ID: **3** Type: **not specified**

Using Soft-X-Rays to study the organization of immune cells: T cells and synaptic contacts

Thursday, 18 January 2024 14:45 (30 minutes)

The metabolic activity of T cells involves the control of cellular proteostasis, including gene transcription, protein translation, de novo protein folding, post-translational modifications, secretion, degradation and recycling. Some of these steps are regulated by the chaperonin complex CCT, which is involved in the correct folding of certain proteins. By limiting CCT levels with siRNA in quiescent cells, lipid composition and metabolic rewiring are altered due to dysregulation of the dynamics of interorganelle contacts, as studied by soft X-ras tomography and fluorescence microscopy. During the activation of T lymphocytes to form immune synaptic contacts, the cytosolic chaperonin CCT (chaperonin-containing TCP1) controls changes in the reciprocal orientation of centrioles and the polarisation of tubulin dynamics induced by T cell receptor activation. These changes ultimately determine the function and organisation of the centrioles, as shown by three-dimensional reconstruction of resting and stimulated primary T cells using cryo-soft X-ray tomography and functional live confocal and TIRF microscopy.

Presenter: MARTIN-COFRECES, Noa (Instituto de Investigación Sanitaria Instituto Princesa)

Contribution ID: **4** Type: **not specified**

Exploring 3D Magnetism through Multi-length Scale Imaging: Unveiling New Frontiers

Thursday, 18 January 2024 15:45 (30 minutes)

Three-dimensional nanomagnetic systems, featuring novel and unconventional spin textures, offer an exciting platform to explore new magnetic phenomena, and also offers possibilities for the development of more efficient, capable and multifunctional technologies. However, harnessing these effects requires an understanding of the fundamental properties and behaviour.
The experimental study of such intricate systems poses a considerable challenge. Until recently, available techniques for probing magnetic materials were confined to flat surfaces or films, rendering the exploration of 3D magnetic systems nearly impossible. As a result, a huge effort has been done in the past few years in the development of state-of-the-art imaging techniques across a range of length scales- from transmission electron microscopy to X-rays- that allows the visualization of the magnetization in three dimensions.
This presentation reviews the developed techniques, showcasing examples that demonstrate how the integration of multiple imaging approaches not only facilitates the study of 3D nanomagnetic systems but also opens avenues for the potential design of complex 3D magnetic devices.

Presenter: RUIZ GOMEZ, Sandra (Max Planck Institute for Chemical Physics of Solids)

Contribution ID: **5** Type: **not specified**

Discussion

Session Classification: Session on Multi-length scale imaging

Contribution ID: **6** Type: **not specified**

Role of ALBA in magnetic molecular materials and devices

Thursday, 18 January 2024 16:35 (30 minutes)

Presenter: CORONADO, Eugenio (Universidad de Valencia)

Contribution ID: **7** Type: **not specified**

New opportunities for pharmacology on Alba II

Thursday, 18 January 2024 17:05 (30 minutes)

Drug development relies on a thorough understanding of the structural parameters governing drug/target interactions and the structural effects resulting from drug binding in the target structure. The Unit for the Development of New Chemical, Biological, and Immunological Drugs aims (among other targets) to design and optimize compounds targeting microtubules, essential cellular polymers crucial for cell division, neuron axon stabilization, and chemical transport. Modulating microtubules is a recognized strategy for targeting cancer, neurodegeneration, and infections. To achieve these goals, we utilize XALOC to analyze drug-protein interactions at the atomic level, NCD-SWEET to examine the effects of drug binding on microtubule structure, and MISTRAL to study the cellular effects of the designed compounds in treated cells.
The advent of ALBA II presents exciting opportunities for pharmacology, providing advanced capabilities and cutting-edge tools for drug development and molecular studies. With enhanced synchrotron facilities, researchers will be able to look deeper into the structural intricacies of drug-target interactions and the intra-cellular localization of the drugs, enabling a more comprehensive understanding of pharmacological mechanisms improving their specificity and optimizing the doses used. The presentation will showcase the outcomes of this multidisciplinary research, highlighting the potential applications and discussing our wishlist for the construction of ALBA II.

Presenter: DÍAZ PEREIRA, José Fernando (CIB-Margarita Salas)

Contribution ID: **8** Type: **not specified**

Challenges and opportunities for machine learning in XAS data interpretation

Thursday, 18 January 2024 17:35 (30 minutes)

The last decade witnessed rapid development in data science and machine learning (ML) methods, which are finding more and more applications across diverse fields, and make a dramatic impact also on the processing of spectroscopic data. In particular, the application of unsupervised and supervised ML methods provides new opportunities for detecting subtle fingerprints of structural changes in working functional materials, processing large data sets from time- and spatially-resolved measurements, and could provide the key also for decoding multimodal spectroscopic data. The deeper integration of the ML into the various steps of data processing pipeline, starting from the first on-the-fly analysis carried out already at the next generation of beamlines, seems to be an imminent future. In this talk we will highlight the need for advanced XAS data analysis approaches, emphasizing the areas where ML could provide a viable solution, and illustrate it with a few recent examples of ML-based operando XAS studies of working electrocatalysts. Nonetheless, as highlighted in this talk, the interpretation of spectroscopic data for realistic functional materials under actual working conditions requires caution, regardless of the data analysis approach implemented. In particular, such materials commonly are mixtures of different species (e.g., passive spectators coexisting with active species), which poses a challenge for such sample-averaging methods as XAS, requiring special care and development of dedicated data analysis tools.

Presenter: TIMOSHENKO, Janis (FHI Berlin MPG)

Contribution ID: **9** Type: **not specified**

Discussion

Session Classification: Session on Multimodal and Big data Approaches

Contribution ID: **10** Type: **not specified**

Mapping the neuronal circuits for smell with light, X-rays and electrons

Thursday, 18 January 2024 18:25 (30 minutes)

Integrating physiology and structure at the neuronal circuit scale can provide a mechanistic understanding on how that circuit works. The glomerular columns in the mouse olfactory bulb contain the first synapse of the olfactory sensory pathway, through a circuit that is compact, modular and accessible to optophysiology setups. A correlative multimodal imaging pipeline that combines in vivo 2-photon microscopy and synchrotron X-ray computed tomography with propagation-based phase contrast provides a robust and versatile approach to identify all neurons imaged in vivo in a multi-mm3 resin-embedded sample of brain tissue. Follow-up targeted imaging is possible with either X-ray nanoholotomography or volume EM, and doing so becomes simpler when milling the sample using a femtosecond laser. Finally, hard X-ray imaging can resolve fine structures in such samples, down to synapses. This approach allows harnessing the resolving power of multiphoton, hard X-ray and volume electron microscopy technologies to create detailed multiscale, multimodal maps of brain circuits.

Presenter: BOSCH PIÑOL, Carles (The Francis Crick Institute, London, UK)

Contribution ID: **11** Type: **not specified**

Role of ALBA in Catalysis

Thursday, 18 January 2024 18:55 (30 minutes)

Commercial like catalysts are very complex systems due to the interplay of different parameters which complicate the understanding of the active site. To this we have to add the dynamic behaviour of the catalyst as well as possible structural catalyst modifications due to reaction conditions which may take place at the surface or even at the subsurface or bulk level of the catalyst influencing its catalytic performance. This talk will discuss the spectroscopic requirements for handling the complexity of actual catalysts using several examples from our joint work with ALBA. The necessity of surface sensitive techniques, multimodal analysis and operando spectroscopic tools under reaction relevant conditions will be specifically taken into account. In the second section of our talk we would like to provide an illustration of how ALBA supports the development of catalysts from basic science to practical application in industry. A few remarks regarding ALBA II involvement in catalysis will be done at the conclusion of the talk, with a focus on nanoscale resolution, multimodal analysis and high pressure spectroscopies.

Presenter: CONCEPCION, Patricia (Instituto de Tecnología Quimica,UPV-CSIC)

Contribution ID: **12** Type: **not specified**

Understanding the performance of halide perovskites by synchrotron based techniques

Thursday, 18 January 2024 19:25 (30 minutes)

Presenter: ANAYA, Miguel (Universidad de Sevilla)

Contribution ID: **13** Type: **not specified**

Discussion

Session Classification: Session on Operando, In-situ and In-vivo/In-vitro environments

Contribution ID: **14** Type: **not specified**

Chemistry and Materials Science example

Contribution ID: **15** Type: **not specified**

Electronic and Magnetic Structure example

Contribution ID: **16** Type: **not specified**

Discussion

Contribution ID: **17** Type: **not specified**

ALBA II Status and Perspectives

Friday, 19 January 2024 09:05 (25 minutes)

Presenter: BISCARI, Caterina

Contribution ID: **18** Type: **not specified**

The upgrade of existing instrumentation

Session Classification: Session on ALBA II Tools

Contribution ID: **19** Type: **not specified**

New beamlines

Friday, 19 January 2024 09:50 (20 minutes)

Presenter: NICOLÀS ROMAN, Josep

Contribution ID: **20** Type: **not specified**

Non X-ray microscopy platform

Session Classification: Session on ALBA II Tools

Contribution ID: **21** Type: **not specified**

Scientific Computing

Friday, 19 January 2024 10:10 (20 minutes)

Presenter: MATILLA BARCELÓ, Óscar

Contribution ID: **22** Type: **not specified**

Battery / Catalysis Laboratory

Session Classification: Session on Partnerships and new ways of interacting

Contribution ID: **23** Type: **not specified**

JEMCA and Planes Complementarios

Friday, 19 January 2024 11:00 (20 minutes)

Presenter: ABALLE ARAMBURU, Lucia

Contribution ID: **24** Type: **not specified**

Integration of institutes

Session Classification: Session on Partnerships and new ways of interacting

Contribution ID: **25** Type: **not specified**

LEAPS

Session Classification: Session on Partnerships and new ways of interacting

Contribution ID: **26** Type: **not specified**

Institutional closing remarks

Friday, 19 January 2024 13:00 (15 minutes)

Contribution ID: **27** Type: **not specified**

Discussion

Thursday, 18 January 2024 19:55 (20 minutes)

Contribution ID: **28** Type: **not specified**

Future of the existing program

Friday, 19 January 2024 09:30 (20 minutes)

Presenter: ATTENKOFER, Klaus

Contribution ID: **29** Type: **not specified**

Partnerships in Spain

Friday, 19 January 2024 11:20 (20 minutes)

Presenters: PALACÍN, M. Rosa (ICMAB-CSIC); OBRADORS, Xavier (ICMAB-CSIC)

Contribution ID: **30** Type: **not specified**

Partnerships in Europe

Friday, 19 January 2024 11:40 (20 minutes)

Presenter: GARCÍA, Gaston (CMAM-UAM)

Contribution ID: **31** Type: **not specified**

Welcome

Friday, 19 January 2024 09:00 (5 minutes)

Presenter: MANSO SILVÁN, Miguel (UAM, Vicerrector de Campus e Infraestructuras)

Contribution ID: **32** Type: **not specified**

ALBA and the Spanish University

Friday, 19 January 2024 12:30 (15 minutes)

Presenters: JAQUE GARCÍA, Daniel (UAM, Vicerrector de Política Científica); MANSO SILVÁN, Miguel (UAM, Vicerrector de Campus e Infraestructuras)

Contribution ID: **33** Type: **not specified**

Session on Multi-length scale imaging, chaired by

Thursday, 18 January 2024 14:45 (1h 30m)

Presenter: MUÑOZ FERNÁNDEZ, INÉS (CNIO)

Contribution ID: **34** Type: **not specified**

Session on Multimodal and Big data Approaches, chaired by

Thursday, 18 January 2024 16:35 (1h 30m)

Presenter: MARTIN GAGO, Jose A (ICMM)

Contribution ID: **35** Type: **not specified**

Session on Operando, In-situ and In-vivo/In-vitro environments, chaired by

Thursday, 18 January 2024 18:25 (1h 30m)

Presenter: CARAZO, José María (CNB-CSIC)

Contribution ID: **36** Type: **not specified**

Session on ALBA II Tools, chaired by

Friday, 19 January 2024 09:30 (1 hour)

Presenter: MIRANDA SORIANO, Rodolfo (IMDEA Nanociencia)

Contribution ID: **37** Type: **not specified**

Session on Partnerships and new ways of interacting, chaired by

Friday, 19 January 2024 11:00 (1 hour)

Presenter: CORONADO, Eugenio (Universidad de Valencia)

Contribution ID: **38** Type: **not specified**

Session ALBA II within Spanish Research Area, chaired by

Friday, 19 January 2024 12:30 (30 minutes)

Presenter: BISCARI, Caterina

Contribution ID: **39** Type: **not specified**

CSIC and ALBA collaborations

Friday, 19 January 2024 12:45 (15 minutes)

Presenter: MARTELL, José María (CSIC)