10:40 AM

(ICACC-S7-010-2024) Advanced magneto-structural characterization of magnetic-based oxide nanocomposites (Invited)

M. Estrader*[1]; A. Roca[2]; A. López-Ortega[3]; R. U. Ichikawa[4]; I. Peral[5]; X. Turrillas[6]; D. del-Pozo-Bueno[7]; M. Varela[8]; S. Estradé[7]; F. Peiró[7]; J. Nogués[2]

1. Universitat de Barcelona, Spain
2. Catalan Institute of Nanoscience and Nanotechnology (ICN2), Spain
3. Universidad Pública de Navarra, Spain
4. Nuclear and Energy Research Institute (IPEN/CNEN-SP), Brazil
5. 5Department of Physics and Materials Science, University of Luxembourg, Luxembourg
6. Institut de Ciència de Materials de Barcelona- CSIC, UAB Campus, Spain
7. LENS-MIND, Departament Enginyeries Electrònica i Biomèdica and Institute of Nanoscience and Nanotechnology of the University of Barcelona (IN2UB), Spain
8. Departamento de Física de Materiales e Instituto Pluridisciplinar, Universidad Complutense de Madrid, Spain

Batteries, electro/photochemical catalysts for energy storage and production are constantly renewed with advanced materials exhibiting higher performance. Within these systems, hybrid materials where each counterpart has dissimilar properties are gaining much interest as synergistic properties may arise. Interestingly, in some cases the external activation of one property might induce changes into the other one, often showing increased performances for the battery/catalytic processes. In the last few years, the magnetic effects of either an external magnetic field or even a magnetic material as the hybrid counterpart of the battery/catalyst has emerged as a hot topic owing to the significant improvement of the respective performances. I will first explain some of these exciting examples. Subsequently I will move into the cases when such hybrid composites fall within the nanoscale and the implications this might have. For instance, for nanocomposites, the structure and composition are often not straightforward to disentangle. Having unknown compositions or phases within a magnetic nanomaterial can hamper the interpretation of the magnetic properties, which are, ultimately, responsible for the improvement of the battery/catalytic processes. Thereby, I will explain and show some examples and the related characterization techniques used at the nanoscale for magnetic-based nanocomposites.

11:10 AM

(ICACC-S7-011-2024) Methane Oxidation Reaction Pathway and Activity of CeO_2 Catalyst with a Variation of Surface Fermi Level: A Multi-scale Simulation Study

S. Ji*[1]; H. Ko[3]; H. Choi[1]; S. Cho[2]

1. University of Cologne, Department of Chemistry, Germany
2. Ajou University, Republic of Korea
3. Korea Institute of Ceramic Engineering and Technology (KICET), Republic of Korea

Catalytic oxidation of methane over CeO2 has been investigated to enhance the reactivity. However, there is still a lack of understanding in greatly changeable catalytic activities of CeO2 even small changes by material engineering e.g. doping or cocatalyst decoration and so on. We studied the underlying mechanism of synergistic catalytic methane oxidation activity change of CeO2 by combining density functional theory (DFT) calculations with mathematical models. Our new theoretical model of surface Fermi level dependent reaction activity enables us to precisely predict reaction activities and pathways of wide band gap semiconductors by explaining how bulk impurity doping and cocatalyst deposition on CeO2 can greatly affect the reactivity in methane oxidation.

11:30 AM

(ICACC-S7-012-2024) Selective placement of modifiers on hematite thin films for solar water splitting

F. L. de Souza*[1]

1. Brazilian Center for Research in Energy and Materials, Brazil

The design of nanostructured materials for photoelectrochemical water splitting relies on a detailed understanding of the reactional bottlenecks. Here, we introduce a single polymeric precursor solution that enables the design of hematite (α-Fe_2O_3) with synergistic bulk and interfacial engineering using trivalent (Al^{3+}, Ga^{3+}), tetravalent (Zr^{4+}, Ti^{4+}, and Hf^{4+}) and a cocatalyst ($NiFeO_x$). The solution causes trivalent to dope hematite lattice to reduce polaronic effects, while simultaneously induces tetravalent enrichment at both surface and grain boundaries, improving charge separation and reducing recombination. Zr^{4+} and Hf^{4+} also led to a refined microstructure derived from interface stabilization, which associated with trivalent bulk doping and $NiFeO_x$ electrodeposition resulted in a photoanode with 65 to 85% of overall efficiency. As a consequence, the modified hematite ultrathin film (176nm-thick) delivered a water oxidation photocurrent of 2.30 to 4.5 mA cm^{-2} in contrast to 0.37 mA cm^{-2} for the pristine system measured at 1.23 V against hydrogen reversible electrode (RHE). The results suggest the simplicity of this new polymeric solution may offer a cost-effective, scalable and versatile alternative for multiple chemical modifications in oxides beyond hematite.

S8 18th Intl Symp on APMT for Structural & Multifunctional Materials & Systems

SYMPOSIUM 8: Advanced composite manufacturing technologies, hybrid processes I

Room: Coquina F
Session Chair: Akihiko Ito, Yokohama National University

8:30 AM

(ICACC-S8-026-2024) Exsolution and Coarsening in Metal-Oxide Systems (Invited)

I. Reimanis*[1]

1. Colorado School of Mines, USA

Microstructure evolution in mixed metal oxides exposed to various redox conditions is important to understand for applications such as catalysis, solid oxide fuel cells, and solar thermal water splitting. In particular, the exsolution and subsequent coarsening of transition metal particles in oxides strongly influence performance. An overview of exsolution and coarsening of Ni in yttria stabilized zirconia and yttria stabilized barium zirconate is provided. Thin films of barium zirconate provide a useful model system to examine the importance crystal orientation in these processes.

9:00 AM

(ICACC-S8-027-2024) Fluidized Bed Chemical Vapor Deposition – a versatile technique for the preparation of ceramic composites

G. L. Vignoles*[1]; N. Bertrand[1]; A. Guette[1]; G. Chollon[1]; H. Plaisantin[1]; S. Couthures[1]; A. El Mansouri[1]; T. Da Calva[1]

1. University Bordeaux, LCTS - Lab for ThermStructural Composites, France

Ceramic composites contain by definition reinforcing phases dispersed in a matrix. One of the sensitive issues of these materials is the compatibility between reinforcements and matrix, during processing and during usage, usually at high temperatures. It is therefore highly desirable in general to provide some protection to the reinforcing phase by a coating. In the case of powders or discontinuous fibers, among other methods, Fluidized-Bed Chemical Vapor Deposition (FB-CVD) is very attractive. Indeed, it is rather versatile and easy to scale up, once it has been suitably controlled. Here we will present some aspects of process engineering necessary