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Name badges:
Name badges will be provided at the registration desk. You will be required to wear your name badges at all times within the Royal Society.
## 10TH MARCH - SESSION 1: The gas/solid interface

*Chair: Stephen Skinner*

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 Grain boundaries as a detrimental interface for the electron mobility in ZnO:Al thin films deposited by atmospheric pressure Spatial Atomic Layer Deposition? A new model to link electrical properties and deposition conditions
David Muñoz-Rojas

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Edouard Querel

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Juande Sirvent

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Federico Pesci
Towards a better mechanistic understanding of electrocatalytic phenomena at oxide / gas interfaces

Juergen Fleig (a)

(a) Institute of Chemical Technologies and Analytics, TU Wien, Vienna, Austria

Solid oxide fuel or electrolysis cells are based on electrochemical reactions at oxide surfaces such as oxygen reduction or water splitting, and the corresponding cell performance depends crucially on the electrocatalytic properties of the electrode / gas interfaces. Also in many other fields the kinetics of oxygen exchange reactions at surfaces is essential, e.g. for sensors or permeation membranes. This leads to much interest in reaction mechanisms of the corresponding reactions. In a first step, often the relevant geometric reaction pathway (via triple phase boundaries or via the electrode bulk) is identified and the most resistive region within the predominant pathway is localized (e.g. a certain interface or the electrode bulk). In a next step, it is desirable to obtain an atomistic understanding of the resistive or electrocatalytic processes. Here, exact surface species or point defects and phenomena such as dissociation or ionization come into play, and despite substantial research activities many questions remained unsolved so far.

This talk presents our recent progress on this topic: Established electrochemical approaches (e.g. Butler-Volmer equation) are often not appropriate for describing such reactions and a novel model was thus developed, which allows a proper interpretation of $p(O_2)$ dependences and current-voltage curves. It is discussed, how composite electrodes can improve the reaction rate by a kind of “job sharing”. Exsolution-based composites are considered at the fuel side (Fe on LSF) and it is discussed, what happens during electrochemical switching of their electrocatalytic activity by an overpotential. Moreover, it is illustrated how nano-particles of Pt on $(La, Sr)FeO_3$ (LSF) thin film electrodes strongly improve the reaction rate of oxygen reduction and also completely change the reaction mechanism and the $p(O_2)$ dependence. Finally, the topic of active sites and electrode degradation is considered, with special emphasis on $(La, Sr)CoO_3$ (LSC) and LSF. Extraordinarily high oxygen reduction activity of pristine thin films is shown, different reasons for degradation are discussed, and surprising defect chemical phenomena are displayed for oxygen evolution from LSC thin films.
**In-situ Probing Catalyst Generation and Deactivation with Ambient Pressure X-ray Photoelectron Spectroscopy**

*Bilge Yildiz*(a,b) *, Jiayue Wang*(a), Alexander K. Opitz*(a,c)*,

(a) Department of Nuclear Science and Engineering, MIT, Cambridge, United States
(b) Department of Material Science and Engineering, MIT, Cambridge, United States
(c) Institute of Chemical Technologies and Analytics, TU Wien, Vienna, Austria

Catalysts design plays a crucial role in both energy storage and fuel synthesis. To enable a precise description of the catalytic reactions, *in situ* characterization of surface chemistry is inevitable. In this talk, I am going to present our recent efforts in using ambient pressure X-ray spectroscopy (APXPS) to understand both the catalyst generation and deactivation under real working conditions.

A recent advance in catalyst design is to exsolve metal nanoparticles at the surface of a supporting oxide. Unlike traditional deposition techniques, the nanoparticle catalysts from exsolution are anchored in the parent oxide, which makes the exsolved nanoparticles more resistant against particle agglomeration. While being a promising pathway, the exsolution efficiency requires further improvement. In the first part of this talk, I will demonstrate the capability to enhance exsolution with biaxial lattice strain on epitaxial La$_{0.6}$Sr$_{0.4}$FeO$_3$ thin films. Coupling surface chemical information from APXPS with morphological information from electron and atomic force microscopy, we found that both surface coverage and dispersion of the exsolved Fe$^0$ particles can be significantly enhanced with biaxial tensile strain.

Regarding catalysts deactivation, carbon deposition from CO and other carbon-containing fuels (“coking”) is a major cause of the performance degradation of catalysts and electrocatalysts in many energy conversion devices. In the second part of the talk, I will present our investigation into the relationship between gas/solid interface compositional and operational factors that lead to the onset of carbon deposition on thin-film CeO$_2$ electrodes at 450 °C in CO/CO$_2$ atmosphere. During the measurement, electrical bias was applied to drive the redox reaction as well as to change surface oxidation state. With *in-operando* APXPS, we tracked the evolution of surface chemical change during carbon deposition on ceria-based thin-film samples. The surface spectroscopy analysis yielded information about the relationship between carbon deposition, surface defect concentration and surface composition.
Intensified catalysis in solid-state electrochemical reactors

Jose Serra (a)

(a) Instituto de Tecnología Química, Universitat Politècnica de València

The gas exchange and catalytic pathways on the surface of solid-state devices is usually determining the evolution rate (nominal current density) but also the selectivity towards different final reaction products and stability of the system. Solid-state ionic materials are a key component in today’s and future energy interconversion as in fuel cells, batteries and electrolyzers. Beyond this application, the application of solid-state ionic conductors in process industry is becoming very relevant and will become indispensable in the transformation of energy to minimize CO₂ footprint via electrification of process units. Electrochemical solid-electrolyte cells enable the design of catalytic reactor processes that shift chemical equilibria favorably and facilitate separation of valued-products. The concept of electrochemically-driven catalytic reactors based on ceramic ion-conducting cells will be presented, where selective electrocatalyst are required to drive the reaction through a preferred pathway, thus, producing selectively a gas product. For instance, protonic membrane reactors allow the intensification of equilibrium-limited reactions where H₂ participates. Ceramic proton conductors based on tungstates or doped BaZrO₃ possess high chemical stability in carbon-containing atmospheres and high proton conductivity. This enables process intensification through integration of the catalytic reactions and separation in one process step, producing pressurized H₂. Beyond equilibrium shift that enables reaching higher per-pass yield of the target product, other remarkable intensification mechanisms can be implemented in the reactor, leading to unprecedented energy efficiency and catalyst stability. One effect is related to the micro-thermal integration at both sides of the solid-state conductor, i.e. by coupling physio-chemical exothermic and endothermic process. Another effect is related to the concomitant transport of oxide-ions through the electrolyte, enabling to control the coke formation or oxidative catalyst decay, depending on the specific process. The overall rate of protons and oxide-ions can be tuned by adjusting the catalytic properties of the electrode. The use of co-ionic assemblies is exemplified in the methane dehydro-aromatization (MDA) process, strongly limited by equilibrium and coking.
Strategies for enhancing oxygen reduction kinetics in SOFC cathodes

Katherine Bagarinao (a)

(a) National Institute of Advanced Industrial Science and Technology, Tokyo, Japan

Novel materials for application as cathodes in solid oxide fuel cells (SOFCs) are currently being investigated to achieve superior electrochemical performance and overcome the sluggish oxygen reduction kinetics at lower operating temperatures. In this presentation, I will discuss some strategies explored by our group to enhance oxygen reduction kinetics in SOFC cathodes, specifically, tuning of cathode microstructures at the nanoscale level and utilization of multilayering approaches to leverage the effect of heterointerfaces on oxygen incorporation.
Thermodynamic treatments of space-charge zones at grain boundaries in ionic solids

Roger A. De Souza (a)

(a) Institute of Physical Chemistry, RWTH Aachen University, Aachen, Germany

In contrast with the bulk phase, an extended defect (dislocation, grain boundary, surface, domain wall) in an ionic solid is not constrained in equilibrium to remain locally electroneutral. Because of interactions between the extended defect and point defects, the extended defect will in general become electrostatically charged, with the adjacent bulk phase concomitantly developing diffuse, enveloping space-charge zones.

The altered concentrations of point defects in these space-charge zones have long been understood to affect, for instance, the transport of charge across grain boundaries in polycrystalline systems. In this presentation, I will draw attention to three aspects that have received far less attention: that space-charge zones can affect the excess Gibbs free energy of a grain boundary [1,2]; that concentrated solid solutions cannot be treated with the standard Poisson–Boltzmann approach [3,4]; and that space-charge zones can provide an unusual contribution to accelerated diffusion along grain boundaries [5]. Throughout the presentation, I will emphasise the need to consider space-charge zones from a thermodynamic perspective.

Solid Electrolytes for Batteries:
Atomic-Scale Insights into Ion Conduction and Grain Boundary Effects

Saiful Islam (a)

(a) Department of Chemistry, University of Bath, Bath BA2 7AY, UK

In the critical area of sustainable energy storage, solid-state batteries are attracting considerable attention due to their potential safety, energy-density and cycle-life benefits [1]. A complete understanding of solid electrolyte materials for lithium- and sodium-ion batteries requires greater fundamental knowledge of their structural, ion transport and interface properties. For example, grain boundary effects on ion transport in oxides versus sulfides are not fully understood on the atomic-scale. This talk will highlight recent studies [2-4] on Li-ion and Na-ion conduction mechanisms, surface structures and grain boundaries in oxide, oxy-halide and sulfide based solid electrolyte materials.

TBA

*Alexander Staykov (a)*

(a) Kyushu University
Understanding the low mobility in ZnO:Al films deposited in oxygen-rich atmospheres thanks to a new conductivity model

David Muñoz-Rojas (a)

(a) Univ. Grenoble Alpes, CNRS, Grenoble INP, LMGP, F-38000 Grenoble, France

Transparent conductive oxides (TCOs) are key components of optoelectronic devices, such as solar cells or LEDs. Aluminum doped ZnO (ZnO:Al) is a promising alternative to currently used ITO (indium tin oxide) since it does not contain scarce indium and can be easily deposited by low temperature, high-throughput methods such as atmospheric pressure Spatial Atomic Layer Deposition (AP-SALD).[1] But ZnO:Al films deposited by SALD present higher resistivity as compared to vacuum chemical and physical deposition methods, such as, ALD, CVD, PLD or sputtering.

In fact, TCOs, and in general all highly doped polycrystalline semiconductors, present high potential barriers and short depletion layers at the grain boundaries. This results in an increased probability of electron tunneling through the grain boundaries, as opposed to the thermionic emission mechanism observed in low doping semiconductors. Existing conductivity models do not properly account for charge tunneling through the grain boundaries in TCOs, which prevents a proper understanding of the scattering mechanisms limiting their conductivity.

We present a new model based on the Airy Function Transfer Matrix Method that allows the numerical calculation of charge mobility through grain boundaries in highly doped polycrystalline semiconductors. The new model has been used to fit experimental data obtained for ZnO:Al samples deposited by AP-SALD and by ALD and sputtering.[2] This has allowed the calculation of the electron trap density at grain boundaries, thus providing the dominant charge scattering mechanisms for the different samples. Our findings help to understand fundamental electrical transport mechanisms in TCOs and provide guidance on how to optimize the deposition conditions. For example, we show that ZnO:Al thin films processed in the open air using AP-SALD contain a high trap density at the grain boundaries due to trapping of oxygen species during deposition. We also show that a simple UV treatment can enhance the conductivity of such films thanks to the light-induced de-trapping of the oxygen species at the grain boundaries.[3]

Interface analysis in the scanning transmission electron microscope

David W McComb \((a,b)\)

(a) Dept of Materials Science & Engineering, The Ohio State University, Columbus, OH 43210
(b) Center for Electron Microscopy & Analysis, The Ohio State University, Columbus, OH 43212

High angle annular dark field (HAADF) imaging in scanning transmission electron microscopy has been extensively used for probing solid interfaces for many years, with many examples of atomic position imaging with picometer precision. The development of direct electron detectors has resulted in new approaches to interface characterization such as 4D-STEM and integrated differential phase contrast that can allow determination of the positions of light elements such as oxygen with similar precision. The same detector technology has delivered vastly improved electron energy-loss spectroscopy capabilities which, when combined with monochromated sources, allow coordination environment, bonding and electronic structure to be probed with much enhanced signal-to-noise ratio. In this contribution I will review these recent developments and illustrate how these new imaging and spectroscopy methods are revealing new insights at interfaces in structural and functional materials.
Interface Engineering and Understanding of Perfect Perovskites from Strongly Correlated Oxides to Ionics

Judith Driscoll (a)

(a) University of Cambridge, UK

Strongly correlated perovskite interfaces have led to emergent effects including the discovery of 2DEGs, new ferroelectrics, magnetics and superconductors, etc. Interface charge transfer, orbital and atomic reconstructions can explain these effects. Interesting interface phenomena also occurs in ionic systems and the question it interesting to ponder whether there is a link to aforementioned effects. In this work, we grow both perfect epitaxial planar superlattice structures and self-assembled vertically aligned nanocomposites to learn about the interfaces in ionic systems. We probe these interfaces using a wide range of characterisation tools and using theoretical calculations. We find that ionic interfaces have both modified ionic conduction (solid-solid interfaces) and catalytic effects (gas-solid interfaces) arising from structural and chemical effects at interfaces.
Self-organised interfaces, crystal chemistry and oxygen mobility in mixed conductors for energy applications

Matthew J. Rosseinsky (a)

(a) Department of Chemistry, University of Liverpool, Liverpool L69 7ZD, UK

It is demanding to achieve the multiple functionality required of an electrode or membrane within a single phase, and hence there has been considerable focus on synthetic composites with interfaces between materials of distinct compositions and structures. Our work has focussed on understanding and controlling the nature of these interfaces. This presentation will address the self-organised assembly of coherent interfaces between isostructural perovskite phases which then co-operate to function as stable low ASR SOFC cathodes (1,2). A range of techniques establish the chemical mechanisms that control the phase separation. The understanding of the mechanisms controlling the interfaces between non-isostructural phases is less advanced, and we have shown that in thin films layer-by-layer two dimensional growth of materials with quite distinct structures can be enforced by considering the extent of chemical bonding as well as geometrical mismatch (3). The strong influence of specific chemical factors on ion mobility and stability under application conditions is demonstrated by the high oxygen mobility and CO$_2$ tolerance of a recently evaluated perovskite containing Bi$^{3+}$. (4)

(2) J.F. Shin et al., Nature Energy 2, 16214, 2017
(3) M. O’Sullivan et al., Nature Chemistry 8, 347, 2016
(4) M. Li et al., Advanced Materials 32, 1905200, 2020
The dynamic metal anode/solid-electrolyte interfaces in solid state batteries

Edouard Querel (a), Rowena Brugge (a), Federico Pesci (a), Andrea Cavallaro (a), Richard Chater (a), Ainara Aguadero (a)

(a) Imperial College London, UK

Safety issues of state-of-the-art liquid flammable electrolytes-based batteries are promoting a race for the successful integration of commercial solid-state batteries in which the integration of metal anodes, opens the door to higher energy and power densities. However, the development of these systems has been so far hindered by the lack of understanding of the dynamic metal/solid interfaces that leads to chemical, electrochemical and mechanical degradation during cell operation.

In this work, we focus on the study of Na/NaSICON and Li/Garnet interfaces using a combination of electrochemical and surface analysis techniques. We prove that the processing conditions can be tuned to optimise the interface chemistry leading to the apparent suppression of the interfacial resistance for ion exchange. The study also proves that the interface is very dynamic leading to both chemical and microstructural changes that can have important effects on the battery cycle life and performance. Our work highlights the complexity of these systems and propose the need of new in situ techniques to gain a deeper understanding of the processes taking place. In this regard, we introduce a novel and beyond state-of-the-art dual secondary ion mass spectrometer (SIMS) aimed at innovative 3D chemical and microstructural analysis with operando capabilities.
Nanomaterials and interfaces for solid state energy microdevices

Albert Tarancon (a)

(a) Catalonia Institute for Energy Research, Sant Adrià de Besòs 08930, Spain

The internet of things (IoT) will revolutionise the way in which we interact with the world around us: sensors of temperature, presence, traffic density will measure data and communicate to a control unit for decision-making. Autonomous actions for process optimization, intervention, environmental safeguard will be taken without human intervention.

Embracing the IoT in our lives will require the advent of a new generation of portable power sources. For this, new families of rechargeable and autonomous micro-energy sources offering high specific power (0.5-10 mW and 1-100 J) have to be developed in order to integrate the required power capabilities in the IoT nodes.

These new technologies will be necessarily miniaturizable and likely based on advanced concepts of Nanoionics and Iontronics, i.e. will take advantage of ion-based local effects at the nanoscale. This way, surprising properties of fast conduction and high storage capacity can be obtained. Moreover, by taking advantage of silicon microfabrication techniques, a superior manufacturability, cost-effectiveness and the possibility to host dense structures in a seamless architecture will be reached; all in an environmentally friendly material.

In this talk, we will present the HARVESTORE project devoted to integrate harvesting and storage units based on new concepts in silicon technology while reviewing interesting concepts of Nanoionics and Iontronics.
Development of Ceres Power’s Steel Cell® technology: The revolutionary power of ceria on steel for multiple global applications

Dr. Subhasish Mukerjee (a)

(a) Ceres Power Limited

Ceres Power is developing and commercializing its low-temperature metal supported SOFC technology (the ‘Steel Cell’) based predominantly around the use of ceria on low cost steel. This unique design architecture allows for a robust, low cost fuel cell product, whilst retaining the advantages of fuel flexibility, high efficiency and low degradation. The technology lends itself to multiple applications in the energy sector.

Over the last few years, several significant technological and commercial developments have taken place. This technology iteration offers higher power, the ability to operate at higher efficiency and state-of-the-art performance degradation rates, whilst retaining the outstanding robustness to thermal cycling, vibration and REDOX cycling characteristic of the Steel Cell technology. Multiple customers and partners are working with Ceres Power to license and develop products for multiple applications globally based on this core technology. This includes customers in Japan, Korea, Germany, China and the USA. This presentation will highlight the progress in the technology, the array of commercial products with this technology and the fast commercialisation of this technology all around the world.
Study of surface oxygen exchange kinetics of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ thin films using Electrical Conductivity Relaxation Measurements

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YBCO films are of great technological interest as they show exceptional good superconducting properties. As in all cuprate superconducting oxides, these properties are governed by the oxygen content of the material. Understanding how to achieve optimal oxygen doping of the oxygen deficient triple perovskite YBCO structure is still an open, critical issue and its optimization a main goal of this work. The oxygenation kinetics is strongly influenced by microstructural and morphological features at the surface. The elementary reaction mechanisms comprise molecular oxygen absorption, ionization, dissociation, incorporation and atomic bulk diffusion.

We show that in-situ techniques as electrical conductivity relaxation (ECR) and high temperature environmental XRD (HTXRD) are very useful tools to analyze the oxygen exchange processes. Thin films studied were obtained by chemical solution (CSD) and pulsed laser deposition (PLD) with thicknesses of 25 to 250nm. We monitor the mechanisms of the oxygen reduction (ORR) and oxygen evolution reaction (OER) in YBCO thin films during post growth thermal treatments by changing between oxidizing and reducing pO2 atmospheres. Our results demonstrate that the ORR in these thin films is limited by surface reactions. This reaction can be catalyzed by sub-micrometer silver particles on the surface.

Further, using a bulk chemical defect model, the pO2 dependence of the surface exchange constant $k_{\text{chem}}$ and the initial reaction rate $\varpi$ allows to identify the rate determining step as the oxygen-oxygen vacancy recombination at the gas-solid interface. Additionally, we find that strain engineering via film-substrate mismatch impacts surface reactions, likely linked to variations in the oxygen vacancy formation energy.

The understanding the oxygen exchange reactions at the surface enables to tune the carrier concentration via the oxygen stoichiometry, leading to remarkable superconducting properties in these YBCO thin films.

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Surface Restructuring of Thin-Film Electrodes Based on Thermal History and Its Significance for the Catalytic Activity and Stability at the Gas/Solid Interfaces

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Electrodes in solid-state energy devices are subjected to a variety of thermal treatments, from film processing to device operation at high temperatures. All these treatments have an influence on the chemical activity and stability of the films, as the microstructure and morphology are shaped by the thermally induced chemical restructuring. Here, we investigate the correlation between the oxygen reduction reaction (ORR) activity and thermal history in complex transition metal oxides, in particular, La\textsubscript{0.6}Sr\textsubscript{0.4}CoO\textsubscript{3-δ} (LSC64) thin films deposited by Pulsed Laser Deposition (PLD). To this end, three ~200 nm-thick LSC64 films with different thermal history were studied; two films were grown at 100 °C and 750 °C substrate temperatures, respectively and the third one was grown at 100 °C and post-annealed at 600 °C for 4 h in ambient air. Oxygen self-diffusion coefficient (\(D^*\)) and oxygen surface exchange coefficient (\(k^*\)) were measured by isotopic exchange depth profiling technique coupled with time-of-flight secondary-ion mass spectrometry (ToF-SIMS). A combination of surface-sensitive elemental characterisation techniques (i.e. low-energy ion scattering; LEIS, X-ray photoelectron spectroscopy; XPS and secondary-ion mass spectrometry; SIMS) were employed to thoroughly investigate the cationic distribution from the outermost surface to the film/substrate interface. Moreover, electrochemical impedance spectroscopy was used to study the activity and the stability of the films. Our research has revealed that the thermal history of films greatly affects the microstructure/morphology and the elemental distribution at the interfaces. However, the degradation rates of the films showed a two-fold difference in the long-term tests, despite initially comparable ORR activity. Here, we emphasise the significance of thermal history particularly for the stability of the LSC64 electrodes and propose that it should be considered as among the main pillars in the design of active surfaces.
New Tools to Analyze the Photoelectrochemistry and other Intrinsic Properties of Ceramic Materials

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Photoconductivity is an important characteristic for any device that relies on a photo-effect. However, it is not easy to distinguish photoconductivity from other effects such as light-enhanced surface exchange or temperature effects. Moreover, the photoconductivity itself can also originate from different charge carriers being excited from different states within the band structure, prone to different recombination mechanisms. Furthermore, temperature itself can modify bandgap, conduction and recombination characteristics. Gaining a full understanding of the processes that generate photoconductivity is not an easy task and involves characterization tools, some of which might require special device architectures and test conditions far from the usual operating conditions.

I will introduce a versatile test setup where model cells can be characterized optically and electrically at the same time, and where important conditions such as temperature, oxygen partial pressure and illumination intensity and wavelength can be varied systematically.

Innovative frequency-domain measurement techniques such as intensity modulated photocurrent/voltage spectroscopy (IMPS/IMVS) are then applied, which have shown to reveal valuable information about charge carrier dynamics for photoelectrodes and photovoltaic cells *in operando* [1]. To the best of my knowledge, these techniques have never been applied for materials characterization as opposed to device characterization. However, with the small signal light perturbation that is the key element of IMPS and IMVS, it is possible to trigger the light effect directly and analyze the different contributions to the system response by well-known impedance analysis tools.

In this contribution, I will give a brief introduction into IMPS and IMVS and show how these techniques can be applied to model electrodes consisting of STO and STF. The results are compared to EIS under different illumination and we will show how to extract the relevant information about the photo-response. By evaluating the activation energies of the different electrochemical and photoelectrochemical processes, we can attribute those to physical effects. With that, we can clarify some of the previously unknown processes that lead to anomalies observed in STO/STF under illumination and obtain valuable information about other intrinsic properties such as band structure.

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Reference
Interfaces and strain in rare-earth substituted ceria: Modifying defect concentrations and mobilities

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There is a coupling between the chemical, electrical, and mechanical properties in electroceramic materials, referred to as \textit{electro-chemo-mechanics}. Therefore, mechanically confined systems such as thin films may be investigated as a route to improved functional properties, shifting the paradigm of materials development away from compositional tuning and searching for new functional oxides. Rare-earth substituted ceria is an excellent model material to study these effects, and in this presentation, we demonstrate two key experimental findings.

First, we demonstrate that the migration barrier in rare-earth substituted CeO\textsubscript{2} can be modified by lattice strain. Using an unconventional approach to straining films, and careful analysis of the literature, we managed, for the first time, to develop a quantitative consensus on the variation in the transport properties of ceria as a function of lattice strain. We also experimentally demonstrate the effects of migration direction with respect to the biaxially strained plane. We find that the modification is dependent on the size of the dopant cation, showing that defect association plays a substantial role. We rationalise our findings using static force-field simulations, suggesting that the cause is due to a combination of changes in the migration barrier and vacancy-cation configuration.

Second, we explore the extent that charge carrier concentrations in mixed ionic-electronic conductors (MIECs) can be modified at interfaces. Pr substituted CeO\textsubscript{2} (PCO) is an excellent MIEC for fundamental studies as it has been extensively investigated, and the defect chemistry, chemical expansion, transport, and optical properties are well described in the bulk material. By fabricating nano-granular polycrystalline films and multilayer heterostructures, we have investigated the effects of homogeneous and heterogeneous interfaces on the concentration of oxygen vacancies and small polarons. Using a combination of impedance spectroscopy in conjunction with \textit{in-situ} optical transmission measurements, to unambiguously extract the non-stoichiometry, we observe substantial deviations from bulk behaviour in materials dominated by a high density of interfaces. By engineering the density and proximity of interfaces, we demonstrate a lowering in the effective enthalpy for Pr reduction, allowing the non-stoichiometry and density of charge carriers to be tailored.
Interface engineering in La$_{0.8}$Sr$_{0.2}$MnO$_{3±δ}$ thin films by tuning local nonstoichiometry in grain boundaries

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Interface-dominated oxides, e.g. in the form of nanocrystalline thin films, have emerged as enthralling systems for energy and information technologies owing to the large tunability of their functional properties. In particular, it was discovered that grain boundaries in manganites are able to deeply impact the overall material’s functionalities by boosting the oxygen mass transport while abating the electronic and magnetic order. In this work, the origin of this remarkable behaviour is assessed. The structural and chemical characterizations of La$_{0.8}$Sr$_{0.2}$MnO$_{3±δ}$ thin films, deposited by pulsed laser deposition, reveal that strained grain boundaries witness a profound modification of the local anionic and cationic compositions. Moreover, it is found that, by tuning the overall cationic content in the thin films (Mn/(La+Sr) ratio), the interface local nonstoichiometry can be purposefully modified, maintaining its oxygen deficiency character yet altering the cationic concentration profiles. Finally, the study of the electrical and electrochemical properties of these interfaces unveils the possibility of tuning the functionalities of manganite thin films by grain boundary engineering.

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Revisiting Lanthanide in Oxides – A Quantum Mechanical Insight into their Catalytic Activities

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Lanthanide containing complex oxides, especially the ABO₃ perovskite and Aₙ₊₁BnO₃n₊₁ Ruddlesden-Popper series, attract much interest as promising catalytic materials in many renewable energy applications such as electro-chemical energy conversion, hydrogen production and chemical looping devices. Recent experimental and theoretical studies on some members of these materials, e.g. La₂NiO₄₊δ, revealed that the La-O terminated surfaces are catalytically active under operational conditions. These findings suggested that the conventional understanding of a fully ionized, catalytically inert La³⁺ ion needs to be revised.

By applying generalized gradient approximation and hybrid density functional theory methods were used to study and compare the electronic structures of representative lanthanides (La, Pr) and alkaline-earth metals (Ba, Sr) in related oxides.¹¹ Consistent results were obtained across different ab initio methods and approaches used. Density of states plots and charge analysis results showed that the lanthanides exhibits a partially occupied d-orbital and a calculated atomic charge of +2 instead of its nominal valence number (+3) in the oxides, while the alkaline-earth metals does not show similar characteristics. Electron density maps obtained from synchrotron X-ray diffraction experiments confirmed the simulation findings as well. The presence of available d-orbital electron on La and associated partial covalency was postulated as being responsible for the catalytic behaviour observed in experiments. Considering the commonality of the lanthanides behaviours in all the simple and complex oxides we studied, we believe that these characteristics should be considered for the general understanding of lanthanides activities in these oxides.

Reference
Ceramic thin film nanocomposites: a playground for energy application

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Self-assembled thin film nanocomposites in the form of vertically aligned nanostructures (VANs) have been intensively investigated in the last years, revealing a plethora of surprising functional properties such as enhanced ionic transport and novel interface electronic states. This is ascribed to the nanoscale phase alternation of the phase components, which allows for interface effects to be predominant over the bulk behavior.

In this contribution, the application of such nanostructures for high temperature electrode application is shown in relation to two relevant cases, namely Sr-doped lanthanum manganite (LSM)/fluorite VANs and mesoporous lanthanum ferrite (LSCF).

In the first example, the structural and electrochemical analysis of LSM/doped zirconia and LSM/doped ceria is presented, highlighting a decisive enhancement of the oxygen reduction kinetics with respect to single phase LSM (about one order of magnitude lower area specific resistance). In the case of mesoporous LSCF, a high-surface structure has been obtained by selectively etching a sacrificial phase from a starting biphasic VAN. The resulting final material exhibits a dramatically reduced activation energy for oxygen reduction reaction (as low as 0.4 eV), which is ascribed to combined microstructural and surface chemistry effects.

Such relevant findings are rationalized via a throughout investigation of the two systems, based on state-of-the-art structural (high-resolution transmission electron microscopy, atom probe tomography, low-energy ion scattering spectroscopy) and electrochemical (impedance spectroscopy) methods.
Layered Ceramic Protonic Electrolyzers Fabricated Via Inverse Tape Casting

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Steam electrolysis via solid oxide electrolysis cell has been demonstrated to be a more efficient method to produce hydrogen using ceramics proton conducting electrolytes. These protonic solid oxide electrolysis cell (P-SOEC) devices can be successfully deployed to reach very high performance in hydrogen production. However, their fabrication techniques are still not yet quite rational at an industrial scale. Upscaling affordable large size (> 50 x 50 mm square) protonic devices meeting commercial targets is very challenging. The fabrication of such multilayered devices usually via a tape casting process requires careful control of shrinkages of individual layers to prevent warping, cracking during sintering.

This talk highlights the successful processing of 5 × 5 cm² planar cathode-supported protonic electrolysis half-cell consisting of Ba(Zr₀.₅Ce₀.₄)₀.₉Y₀.₂O₂.₉ electrolytes, a functional NiO-SrZr₀.₅Ce₀.₄Y₀.₁O₃-₅ cathode layer and NiO-Ba(Zr₀.₅Ce₀.₄)₀.₉Y₀.₂O₂.₉ substrate using an inverse tape casting route. The smooth tri-layered green tapes produced, yielded suitably dense and gas-tight electrolyte layers after co-sintering at 1350 ºC/5h. Current-voltage characteristics and hydrogen evolution rates measured in the temperature range 500-600°C, using Ba₀.₅La₀.₅CoO₃-δ as anode, demonstrate excellent performance and durability. Electrolysis voltage as low as 1.2 V are attainable at current densities of 0.2, 0.4 and 0.5 A/cm² at 500, 550 and 600 °C, achieving faradaic efficiencies close to 100% in the later, which is among the best PC-SOECs performance reported in literature. Microstructural optimized cells as well improvements in current collection also yield a current density of 1 Acm² at 600 °C at an operating voltage of 1.36 V. Beside electrochemical characteristics, the morphology of the tri-layered half-cells were also analyzed by a combination of high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) and energy-dispersive X-ray spectroscopy (EDS). We observe the precipitation of Y₂O₃ and substantial amount of Sr and Ba inter diffusion as well as Ni migrates in the vicinity of NiO grain and the electrolyte interface for all half-cells sintered at 1500 ºC.

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References
Hydration in BaLnLn’Co$_2$O$_{6-\delta}$ cobaltites – a wide perspective.

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The cobaltites with perovskite-related structures are promising candidates for positrodes for SOFCs and SOECs. The general formula of investigated materials is BaLnLn’Co$_2$O$_{6-\delta}$ (Ln, Ln’ = La, Pr, Nd, Sm, Gd, Tb, Dy or Lu). In this system, different structures, starting from cubic (space group Pm-3m) to layered perovskites (e.g. space groups P4/m or Pmmm) can be adopted depending on the ionic radius of the lanthanide and the oxygen content. In some cases also superstructures may be formed.

In the last decade numerous oxides, that exhibit proton conductivity, have been introduced and extensively studied by multiple techniques unrevealing both transport properties and proton uptake thermodynamics. One of the most direct investigation methods designed to determine the latter is thermogravimetry (TGA). Two major types of study used to determine water uptake are switches from dry to humid atmosphere in the isobaric or the isothermal mode. In the case of barium lanthanide cobaltite, the isothermal approach proved to be suitable in contrary to isobaric approach. The quantification of the protonation level should take into consideration all possible processes that can be associated with water incorporation including hydration, hydrogenation, oxygenation and hydroxidation. In this work, the water uptake of multiple compositions from BaLnLn’Co$_2$O$_6$ system has been analyzed.

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