



Impact of processing on the Fermi-level of advanced electroceramics

International Workshop, March 3–7, 2024,
Seeheim (Germany)

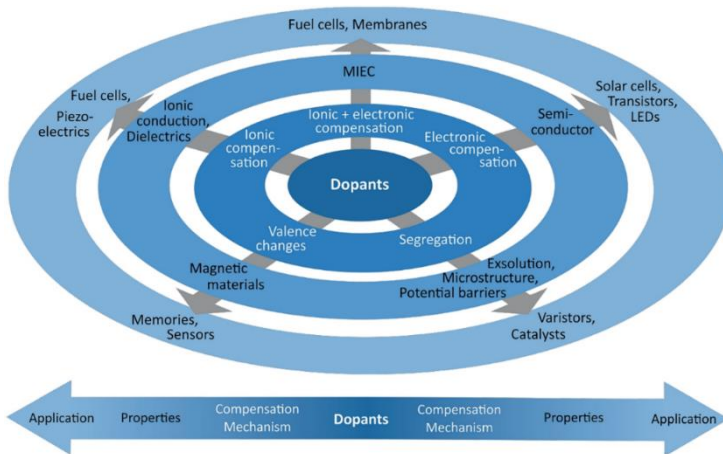


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Welcome Address

Oxide electroceramics are well established materials. Their catalytic, electric, dielectric and electromechanical properties make them suitable for a variety of different applications including capacitors, solid oxide and proton conducting fuel cells and membranes, memories, sensors, and piezoelectric transducers. The properties of electroceramic oxides can be adjusted by doping and chemical substitution. Depending on the host material and the dopants, the resulting properties are determined by how the charges introduced by doping are compensated. All possible charge compensation mechanisms



can be described by the dependence of the involved defects on the Fermi energy. Understanding and quantifying the properties will allow to compare the different compensation mechanisms on the same energy and should enable us to predict the prevailing compensation mechanism and eventually material properties for given compositions. The precise control of material properties by engineering the

Fermi energy is a reality for semiconductor technology. The Collaborative Research Center FLAIR, which has been established by the German Research Foundation in 2023, is aiming at applying the concept of Fermi level engineering to oxide electroceramics.

As part of this effort, the **First International FLAIR Workshop** will bring together the members of FLAIR and international experts from different fields to discuss specifically the connection between the Fermi energy and issues related to material processing and properties. Such a connection is expected as thermodynamic phase stability is related to the chemical potentials of all involved species, including those of the electrons. The workshop will present invited talks and provide ample of time for scientific discussions.



Andreas Klein



Karsten Albe

Chairs of the Workshop

Conference venue

The [Lufthansa Seeheim Conference Hotel](https://www.lh-seeheim.de) is located approximately 45 km south of Frankfurt am Main in a pleasantly inspiring setting – at the heart of the Bergstraße-Odenwald Nature Park. There is a [shuttle](#) service between the hotel and the airport (and its long-distance train station). The trip takes around 35 minutes. The bus arrives at and departs from bus platform 23 on the arrivals level of Terminal 1A.



<https://www.lh-seeheim.de>

How to get there

Arrival by car

The hotel is easiest to reach by car from the exit No. 28, Seeheim-Jugenheim, of the A5 Autobahn (roughly halfway between Frankfurt and Heidelberg). Satnav data: Seeheim-Jugenheim, Lufthansaring 1. Parking facilities are free of charge in the underground car park.


Arrival by plane

For attendants arriving by plane or train, there is a [shuttle service](#) free of charge from the bus station at Frankfurt Airport (bus stop platform 23 in front of Terminal 1, arrival area A), which takes about 35 minutes.

Arrival by train

From InterCityExpress train station at Frankfurt Airport, please use the [shuttle bus](#) (see arrival by plane). From Frankfurt main train station (Hauptbahnhof), you can take the S-Bahn, line 8 or line 9 to the airport Frankfurt, and then the shuttle bus. Alternatively, you can take the regional train to Bickenbach station and continue from there via taxi.





Programme and Abstracts

The programme starts on Sunday night with a dinner and a welcome in the bar. Talks are scheduled in a way that provides enough time for discussions. In the JuniorFLAIR sessions, young FLAIR researchers will give insights into their current work on the CRC. On Tuesday, we will have a walk to the nearby Schloss Heiligenberg. A guided tour will inform about the surprising history of the place and its former inhabitants. In the evening, we return to the Lufthansa-Center for dinner.

Sun.	Monday	Tuesday	Wednesday	Thu.
	Session 1 Electronic Structure	Session 5 Defects and Devices		Session 7 Materials Chemistry 1
9:00	1-1 Klein	5-1 Lany	9:00	7-1 Rosseinsky
9:40	1-2 Chambers	5-2 von Wenckstern	9:40	7-2 Clemens
10:20	Coffee & Tea			
	Session 2 Piezoelectricity	Session 6 (Photo)electrochemistry		Session 8 Materials Chemistry 2
10:50	2-1 Rheinheimer	6-1 Streibel	10:50	8-1 Scavini
11:30	2-2 Einarsrud	6-2 Risch	11:30	8-2 Widenmeyer
12:10	2-3 Iacomini	6-3 Hofmann	12:10	8-3 Maibach
13:00	Lunch			
	Session 3 JuniorFLAIR 1	Excursion to Schloss Heiligenberg		Session 9 JuniorFLAIR 2
14:30	3-1 Chaoudhary		14:30	9-1 Barroso
14:45	3-2 Cichocka		14:45	9-2 Neumann
15:00	3-3 Paulik		15:00	9-3 Sehwat
15:15	3-4 Kunz		15:15	9-4 Wang
15:30	Coffee & Tea		15:30	9-5 Kang
			15:45	9-6 Kler
	Session 4 Defects		16:00	Coffee & Tea
16:00	4-1 Fleig			Session 10 Wrap-up & Outlook
16:40	4-2 Merkle		16:40	10-1 Albe
17:20	4-3 Gunkel	17:20	10-2 Feedback, discussion, outlook	
18:00	4-4 discussion	18:00		
19:00	Dinner			

MONDAY

Session 1 | *Monday 4.3.* | 9:00–10:20
Electronic Structure | Chair: Karsten Albe

1-1 | 9:00

The Fermi energy and sample processing

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The Fermi energy in materials is generally determined by charge neutrality. As long as materials are pure and perfectly stoichiometric, charge neutrality is fulfilled. Charges arise if dopants are added or if a material becomes non-stoichiometric. Non-stoichiometry on the anion site depends on the gas atmosphere. A cation non-stoichiometry during sample processing can result from the volatility of species or from different solubilities during the formation of solid solutions. In any case, synthesis of targeted phases is relying on the ability of materials to compensate the charges arising during their processing. Charge neutrality can, for example, be established by the addition of electronic charges in the valence or conduction band. This is not always possible, for example in insulators. In the case of oxides, materials can exchange oxygen with the surrounding atmosphere. In

some cases, the only remaining possibility is to change the cation content, which often leads to the formation of secondary phases. The appearance of secondary phases can therefore indicate that charge neutrality is difficult to adjust in the targeted material. We expect that this is caused by the Fermi energy approaching the limit of thermodynamic stability. In order to improve sample processing, it is, therefore, crucial to consider and eventually overcome Fermi energy limitations. The presentation will introduce the different mechanisms, which can limit the Fermi energy, how these could be related to sample processing and how these can be determined by means of photoelectron spectroscopy.

1-2 | 9:40

Fermi level engineering and evolution in epitaxial complex oxide heterostructures

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The Fermi energy relative to band edges at interfaces and within individual layers is of critical importance in determining the electronic properties of complex oxide heterojunctions. Many metal oxides exhibit electronic properties that can be at least partially controlled by doping. However, unlike heterostructures consisting of conventional group IV and group III-V semiconductors, those involving complex metal oxides often contain non-negligible concentrations of defects that can exert a major influence on the Fermi energy throughout the system. The most prevalent are cation and oxygen vacancies along with anti-sites that can result from cation mixing when there is high solubility at interfaces, or inaccurate flux

calibration during film growth. While materials engineering based on rational doping schemes is certainly useful in designing functional oxide systems, the presence of these point defects can alter materials properties in unexpected and interesting ways. It is thus essential that the interplay between intentional dopants and point defects arising from the many degrees of compositional freedom in complex materials be understood to enable the informed design of materials systems.

In this talk, I will give an overview of our work on the use of x-ray (both soft and hard) and ultraviolet photoemission, along with x-ray absorption spectroscopies, in determining energy profiles of complex oxides heterostructures synthesized by means of molecular beam epitaxy. Examples will be taken from the realms of p - $\text{Sr}_x\text{La}_{1-x}\text{CrO}_3/n$ - $\text{SrTiO}_3(001)$ [1-4] and n - $\text{SrTiO}_3/\text{Si}(001)$ [5-10] in which Si (STO) dopants include O, P and Al (V_O , Nb, La and Yb). The information from these spectroscopies nicely complements electronic transport measurements and together these two modalities, along with first principles modeling, yield deep insight into the physics, chemistry and electronic properties of these heterostructures.

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Session 2 | Monday 4.3. | 10:50–12:50
Piezoelectricity | Chair: Jürgen Fleig

2-1 | 10:50

Interplay of defects and microstructure evolution in perovskites

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Perovskite ceramics are widely used in a variety of electronic devices, e.g. capacitors, oxygen conductors, PTC (positive temperature coefficient) heaters and piezoelectric actuators. Many macroscopic properties of polycrystalline perovskites are governed by defects and their interplay with grain boundaries during processing.

This presentation investigates the impact of defects on sintering and grain growth. Strontium titanate was chosen as a perovskite model system. One focus is on the role of point defects in grain boundary migration: using defect-chemical parameters such as oxygen partial pressures and electric fields, the importance of space charge and solute drag for microstructure evolution is underlined.

A second focus is the interplay of processing and dislocation-based plasticity. It is shown that a high heating rate during sintering can result in the nucleation of dislocation and, subsequently, in a high dislocation-mediated plasticity, which is very unusual for ceramics.

These findings were used to invent a new sintering technology for ceramics: blacklight sintering, where UV-rich light is used to sinter ceramics within seconds to full density. This technique bears immense economic potential due to its convenience, speed and low energy need.

2-2 | 11:30

Tailoring electroceramic materials properties through wet chemical synthesis

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Aqueous chemical solution-based synthesis methods are a simple, environmentally-friendly, and up-scalable processes to oxide electroceramics for different applications. The synthesis methodology is based on a solution containing a homogeneous stoichiometric mixture of precursors, followed by annealing, and finally crystallization. The synthesis approach facilitates easy addition of dopants and due to the homogeneous mixing of elements already in the solution, metastable phases can be synthesized. High quality materials produced in a reproducible way are needed for Fermi level engineering of electroceramics and we have developed a unique set of in situ characterization units to reveal precursor decomposition, nucleation and crystallization mechanisms to aid in materials development. Our in-situ characterization platform includes a cell for

synchrotron X-ray diffraction studies of the annealing and crystallisation steps during the aqueous chemical solution deposition of thin films, a unit for synchrotron X-ray diffraction and total scattering during hydrothermal synthesis and an in situ IR spectroscopy cell. Using this information, we can tailor materials structure, dopant level, orientation, and properties. Here we report on guidelines for how to design fabrication of oxide electroceramics including lead-free piezoelectric materials as powders and thin film. This understanding will guide us to design of the optimal reproducible procedure for fabrication and tuning the desired materials properties.

2-3 | 12:10 am

Tuning the electrical conductivity and Maxwell-Wagner relaxation in 0.67BiFeO₃-0.33BaTiO₃ piezoceramic prepared by mechanochemical activation

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Since their initial discovery in 1959, lead-based relaxor ferroelectrics, such as Pb(Mg_{1/3}Nb_{2/3})O₃-PbTiO₃ (PMN-PT), have garnered significant attention due to their remarkable electromechanical properties [1]. However, the shift towards "lead-free" material systems necessitates the replacement of PMN-PT and other Pb-based relaxors. Among the "lead-free" ferroelectric materials, the BiFeO₃-BaTiO₃ (BFO-BT) system with a morphotropic composition (~67% BFO) stands out as one of the most promising, exhibiting appealing piezoelectric properties (>110 pC/N) and a high Curie temperature (>400 °C) [2].

However, the current challenges associated with BFO-BT can be attributed to two main factors: i) heterogeneous composition characterized by core-shell structures and secondary phases, and ii) the extensive use of the quenching method to improve piezoelectric properties. The latter often results in metastable properties, with quenched samples consisting of kinetically locked disordered defects that tend to revert to their equilibrium ordered positions over time and with thermal energy [3]. Addressing these issues requires defect engineering of the BFOBT system, which necessitates a systematic study of the point defects within this ceramic. In this context, this research focuses on the synthesis and study of point defects in BFO-BT ceramics prepared through mechanochemical activation (MA). MA proves to be a simple and effective method for producing high-quality BFO-BT ceramics with high densities (>93% of theoretical density) and minimal core-shell structures and secondary phases. Overall, this study provides insights into optimizing the performance of ferroelectric materials through targeted annealing and doping strategies, shedding light on the potential for improving the overall functionality of BFO-BT ceramics.

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Session 3 | Monday 4.3. | 14:30–15:30
JuniorFLAIR 1 | Chair: Joe Kler

3-1 | 14:30

Operando XPS studies of electrodes and electrolyte/electrode interfaces of solid oxide electrochemical cells

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The change of the oxygen content in a material using an electrochemical cell is an important asset to understand the variation of the Fermi energy in materials, paving the way for Fermi level engineering as a versatile toolkit for designing a broad range of materials according to specific applications. The electrochemical cell is constructed by top and bottom electrodes deposited on an oxygen ion conducting electrolyte. The reduction or increase of the oxygen content in the electrodes by cathodic or anodic polarization is accompanied by an increase or lowering of the Fermi energy, respectively. The latter can be monitored together with chemical changes of the sample if the electrochemical cell is operated in an X-ray photoelectron spectrometer. We will present experiments using Y-stabilized zirconia, Fe-doped SrTiO₃, or (anti-)ferroelectric perovskites as electrolytes, and (Sn-doped) In₂O₃, SrFeO_{3.6} and Sr-doped LaCoO_{3.6} as electrode materials. The use of the setup to quantify the Fermi energies of charge transition levels in either the electrolyte or the electrode will be demonstrated.

Electron diffraction techniques for *ab initio* structure determination

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Perovskites (ABX_3) and perovskite-related compounds are some of the most chemically diverse crystal structures with many possible substitutions at A and/or B sites, as demonstrated in oxide systems [1,2]. These materials can be produced using facile processing techniques and yield high performance devices, although they are characterized by large compositional and structural heterogeneities at multiple length scales.

Heterogeneity, especially at the nano and microscale, is key to understanding some of the critical questions on performance and stability. Characterization techniques, such as scanning electron diffraction (SED) or three-dimensional electron diffraction (3D ED) [3,4] are particularly advantageous, because they allow access to the relevant nano- and microscales. Both of these advanced electron diffraction techniques are beneficial to understand the compositional and structural information of perovskites.

In this talk, I will present the unique advantages in studying crystalline materials by using electron diffraction methods.

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3-3 | 15:00

First step towards co-doping of $\text{Ba}_x\text{Ca}_{1-x}\text{Zr}_y\text{Ti}_{1-y}\text{O}_3$ piezoceramics: Understanding the reaction route during solid-state synthesis

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$\text{Ba}_x\text{Ca}_{1-x}\text{Zr}_y\text{Ti}_{1-y}\text{O}_3$ (BCZT) is a ferroelectric material system, which is characterized by its outstanding piezoelectric coefficients and high dielectric permittivity [1,2]. To make this system viable for specific applications, the dielectric properties need to be tailored through aliovalent doping. The long-term aim of this project is to use Fermi level engineering [3] to explore and quantify the effect that acceptor-donor-co-doping has on the defect states, electronic structure, microstructure, and finally dielectric and piezoelectric properties of BCZT perovskite ceramics.

The first step towards understanding of dopant effects is the preparation of high-purity BCZT with low/controlled amounts of impurities. This requires detailed knowledge of phase formation mechanisms and reaction kinetics during solid state synthesis of this complex solid solution, which is not available to date.

To this end, we carried out an ex-situ X-ray diffraction study of the solid-state reactions during formation of the $\text{Ba}_{0.82}\text{Ca}_{0.18}\text{Zr}_{0.08}\text{Ti}_{0.92}\text{O}_3$ composition, complemented by thermogravimetric analysis and granulometry. The intermediary phases have been identified and the reaction route was determined. Scanning electron microscopy with energy dispersive X-ray spectroscopy analysis has been used to characterize secondary phases in undoped, *A*-site-excess, *B*-site-excess, and Fe-acceptor-doped sintered samples.

We found that simple perovskite structures of the individual constituents and $A_2\text{BO}_4$ -structured phases form during solid-state synthesis. CaTiO_3 forms late in the process, but remains as a secondary phase, possibly due to solubility limits. Polytitanate secondary phases appear as well, and were found to be rich in Fe in the doped samples. The amount of secondary phases was reduced by adding excess *A*-site-cations to the system. These findings improve our understanding of the formation reactions and provide the knowledge necessary to identify the origin of secondary phases in co-doped samples.

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Topochemical modifications of Ba-rich perovskite oxide materials

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Perovskite compounds ABO_3 are known for their structural and compositional flexibility on the cation A and B site as well as on the anion sublattice. The introduction of anions in the host lattice modifies the chemical properties, because of their impact on the transition metal oxygen bond as well as on the oxidation states of the B cations. Typical application fields for mixed anion perovskite structure types are for example as magnetoelectric and catalysts.

In this contribution we investigate systematically the structural changes of Ba-rich transition metal oxides $BaFe_{1-x-y}Co_xTi_yO_{3-d}$ under different reaction atmospheres and synthesis routes. The structure of newly synthesized perovskites is tunable by the given ratio of transition metals. Furthermore, we investigate the effect of topochemical fluorination of $BaFe_{1-x-y}Co_xTi_yO_{3-d}F_z$ with increasing amount of fluorine ($z = 0.34; 0.5$). For the fluorination of Ba-rich transition metal oxides a topochemical reaction route was employed with a maximum temperature of 370 °C and PVDF as fluorination agent. Structural changes induced over the amount of fluorine combined with a different ratio of B site cations reveal a complex competition between anion ordering, structural rearrangements, and thermodynamical stability.

4-1 | 16:00

**Fermi levels in mixed conducting oxides:
How they affect space charges, battery electrode potentials
and oxygen exchange kinetics**

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Mixed ionic and electronic conductors (MIECs) are often characterized by a non-trivial interplay of ionic and electronic defects. This interplay causes interesting phenomena which can be exploited in numerous applications, e.g. ambipolar diffusion of formally neutral species in solid oxide fuel cell electrodes or chemical charge storage in intercalation battery electrodes. However, a lack of detailed understanding leaves it partly unknown how specific materials changes are related to the corresponding electrode properties. For example, it is far from trivial to quantitatively predict the effect of the Fermi level on electrode properties in oxide semiconductor devices, batteries or solid oxide fuel and electrolysis cells.

In this talk, highly conducting MIECs such as $(\text{La,Sr})\text{FeO}_3 = \text{LSF}$ or $(\text{La,Sr})\text{MnO}_3 = \text{LSM}$ are considered in three different applications: First, space charges in SrTiO_3 single crystals are induced by LSF/LSM thin film electrodes and investigated by impedance spectroscopy, tracer diffusion, XPS and photo-voltage measurements. A model is developed, which explains the interplay of ionic and electronic

defects in determining the space charge potential. This model also reveals how the reducibilities of the materials (i.e. the energetics of oxygen release) are related to the corresponding space charge potentials. In the second part, MIECs such as LSF and LSM are used as electrodes in oxygen ion batteries. The empirical charge-discharge curves as well as the absolute electrode potentials are discussed in terms of defect chemical models (Brouwer diagram, Fermi level) and chemical capacitance measurements. Finally, these MIECs are employed in their main field of application, namely as electrodes in solid oxide fuel and electrolysis cells. The effect of the Fermi level on the kinetics of the oxygen exchange reaction is discussed. It is shown that Fermi level changes (overpotentials) usually act via defect concentration changes rather than by electrostatic potential changes (space charges). Models are presented to quantify oxygen exchange reaction rates and it is demonstrated how mechanistic conclusions can be drawn from measured bias voltage and partial pressure dependences.

4-2 | 16:40

Mixed-conducting barium ferrate perovskites: proton concentration and mobility

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Triple-conducting oxides containing mobile oxygen vacancies, protons, and electronic defects are key functional materials, e.g. as cathode for protonic ceramic fuel cells where the protonic conductivity is decisive to activate the whole cathode surface for the

oxygen reduction reaction. A minor proton conductivity may also be present in oxides not deliberately designed as proton conductors (such as memristor materials) and modify their functional properties.

Triple-conducting perovskites such as $\text{BaFeO}_{3-\delta}$ typically show lower degrees of hydration than $\text{Ba}(\text{Ce,Zr,Y})\text{O}_{3-z}$ electrolytes.[1,2] The reasons are elucidated from experiments (thermogravimetry, x-ray absorption spectroscopy XAS) and density functional theory (DFT) calculations.[3,4] DFT results confirm the importance of Fe-O covalency for the materials properties. Electron holes are largely found in oxygen states and thus strongly affect the hydration reaction. The transition from electrolyte-type to mixed conductors will be discussed on the example of the $\text{Ba}(\text{Zr,Fe,Y})\text{O}_{3-\delta}$ solid solution, in which already a Fe content in the range of 10% strongly decreases the hydration.

Proton migration in BaFeO_3 occurs with the same phonon-assisted mechanism as in $\text{Ba}(\text{Ce,Zr,Y})\text{O}_{3-z}$ electrolytes, i.e. a preceding $\text{O}^{\cdot\cdot}\text{O}$ approach provides the suitable geometry for the actual proton transfer.[5] Interestingly, oxygen deficiency and correspondingly decreased formal Fe oxidation state lower the proton migration barriers.

Overall, the $\text{Ba}(\text{Zr,Fe,Y})\text{O}_{3-\delta}$ materials family demonstrates the close interrelation of geometrical and electronic structure (buckling of Fe-O-Fe connections decreases the Fe-O covalency), and illustrates the effects on proton concentrations (increased basicity of oxygen and higher proton concentration) and mobility. These relations can then be applied for a targeted optimization of functional materials.

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4-3 | 17:20

Fermi level during ion-triggered metal-insulator transitions in complex oxides

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Complex oxides have evolved as a major class of functional materials applied in a wide range of energy conversion and storage approaches as well as electronic devices, which harvest the ability to precisely tailor and combine oxides on the nanoscale. Here, miniaturization and confinement phenomena can occur that determine the ionic-electronic structure of oxide thin films, surfaces, and interfaces. Moreover, complex oxides can often undergo intrinsic transitions in electrical conductivity which can vary by orders of magnitude or even show true metal-insulator transitions depending on their specific defect structure.

From a semiconductor picture, such conductivity variations and metal-insulator transitions should be accompanied by a relative shift of the Fermi level with respect to the valence band. However, a more complex behavior is often observed in oxides due to the multitude of variable defect concentrations which often yield complex co-doping

scenarios. Moreover, in confined dimensions dopants may redistribute spatially, leading to a separation of ionic and electronic charge carriers and the formation of space charge layers.

Here, we will discuss the implications of such complex defect scenarios on the behavior of the Fermi level in SrTiO₃ thin films, heterostructures, and interfaces, with a particular perspective on the relative shift of the Fermi level observed by means of in-situ (ambient pressure) photoemission spectroscopy. We furthermore address the spectroscopic fingerprint of the oxygen-ion-exchange triggered metal-to-insulator transition in (La,Sr)CoO₃ under reduction. Here, the structural transition from perovskite to brownmillerite structure coincides with a significant shift of the Fermi level with respect to the oxygen 2p band centers, indicative of an electronic transition into the insulating state.

4-4 | 17:50

Discussion

TUESDAY

Session 5 | *Tuesday 5.3.* | 9:00–10:20

Defects and Devices | Chair: Jan Philipp Hofmann

5-1 | 9:00

Defect equilibria from first principles: From widegap oxides to topological semimetals

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Materials functionality and performance is rarely determined by the ideal crystal alone but is usually affected by formation of imperfections and the solution of impurities. In some applications, such as solar thermochemical hydrogen generation, defect formation is the fundamentally enabling mechanism of the desired functionality. In other cases, such as Cd_3As_2 topological semimetals, unintentional self-doping presents an obstacle to the access to the unique electronic properties. In either case, a quantitative understanding of the relevant defect mechanism is essential for developing design strategies. This presentation will touch upon numerous aspects in the computational simulation of defect equilibria, including non-equilibrium design strategies, the coupling of solid state and gas-phase reactions, dopant-defect and defect-defect interactions, both attractive and repulsive, the accuracy of

total energy functionals and electronic structure methods, and the role of the shape of the density of states for the charge balance condition and Fermi level position, as well as machine-learning prediction of defect energies [1]. Specific materials systems include Ga_2O_3 [2], Cd_3As_2 [3], and $(\text{Sr,Ce})\text{MnO}_3$ [4].

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5-2 | 9:40

Current Status and Perspectives for the Creation of Material Libraries by Combinatorial Pulsed Laser Deposition

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The discovery of new functional materials by exploring the phase space of multinary alloys is greatly accelerated by high-throughput experimental and computational screening methods. On the experimental side, high-throughput screening requires sample sets with a systematic variation of chemical composition. This can, among other methods, be achieved by combinatorial pulsed laser deposition (C-PLD) to create spatially addressable material libraries to be analyzed with spatially resolving physical property screening methods for high-throughput characterization [1]. We will summarize the history and current status of C-PLD and discuss in detail the use of segmented targets to realize material libraries composed of, e.g., the

group III sesquioxides [2] or copper halides [3]. Group III sesquioxides are promising materials for applications in next-generation high-power electronic devices [4]. We address the physical properties of various polymorphs of $(\text{Al,Ga,In})_2\text{O}_3$ as a function of cation composition. As another example, the physical properties of a discrete composition spread material library of $\text{Cu}(\text{Br,I})$ are presented as a function of the anion composition. Finally, novel routes and perspectives such as MARS-PLD, a shadow-masked-based approach to area-selective deposition by PLD [5], or the application of C-PLD to study the exsolution of metallic particles from a perovskite oxide matrix are discussed.

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6-1 | 10:45

Designing Transition Metal Oxynitrides for Photoelectrochemical Applications

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Transition metal oxynitrides are an emerging class of functional materials with tunable electronic and optical properties. They offer a high potential for tailored materials development since their Fermi levels, energy band gaps, valence/conduction band positions, and surface chemistry can be controlled by adjusting the cation and anion composition. These design opportunities are especially important for photoelectrochemical applications. In this contribution, I will discuss our group's approach to developing transition metal oxynitride thin films as photoelectrodes using reactive sputter deposition. First, I will discuss the influence of the anion ratio, focusing on the zirconium oxynitride system. As we introduce controlled amounts of oxygen at otherwise fixed deposition conditions, we observe a transition from metallic ZrN to a disordered nitrogen-rich Zr_xN_y to a crystalline bixbyite-type Zr_2N_2O to nitrogen-doped cubic ZrO_2 . At sufficiently high oxygen concentrations, we observe the opening of a band gap in the UV-visible range and the emergence of photoelectrochemical activity for oxidation reactions. Second, I will focus on cation substitution using the example of the titanium tantalum (oxy)nitride system [1]. For this system, we demonstrate that controlled Ti-doping of Ta₃N₅ thin films dramatically reduces their concentration of deep-

level defects and thereby enhances their photoelectrochemical activity.

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6-2 | 11:30

Role of the Fermi level in oxygen electrocatalysis and its measurement using X-ray spectroscopy

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The Fermi level is the electrochemical potential of electrons. It determines which states in a given electronic structure participate in charge transfer and as such is an important property to understand the mechanisms of electrocatalysis and electrocorrosion of electrocatalytic materials. [1] The current discussion in the electrocatalytic literature is focused on rationalizing trends of electrocatalytic reactions based on adsorption properties and derived properties where facile electron (and coupled proton) transfer is assumed. [2] The latter assumption may not be fulfilled for semiconductor electrodes. [3] I will discuss and show examples where the relative Fermi levels of perovskite oxides and typical alkaline electrolytes before contact lead to blocking of electron transfer, e.g., via band bending, and where electron transfer is unimpeded. [2,4,5] These examples highlight the need for Fermi level engineering for optimization of semiconductors used for oxygen electrocatalysis.

X-ray absorption spectroscopy (XAS) probes the unoccupied electronic states so that spectral intensity is at or above the Fermi level. [6] This

enables tracking relative changes in the Fermi level when changes in the density of states are negligible. Transmission- or fluorescence-based XAS can be performed in the presence of sizable liquid layers or even (modified) devices which makes the method ideally suited to resolve changes in the Fermi level upon contacting semiconductors and electrolytes of various compositions as well as with applied triggers (potential, photo-excitation). XAS probes the bulk but differential approaches or grazing incidence emphasize the response from near the semiconductor-electrolyte interface. [7,8] This makes it an attractive tool to investigate the role of relative changes in Fermi level on electrocatalytic reactions.

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Interface chemistry and energetics of oxide photoelectrodes for solar water splitting

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Sustainable energy storage and conversion is key for the transition to a CO₂-neutral energy system. In the required transition technologies, solar energy conversion to and storage of the intermittently available electricity in chemical bonds, i.e., solar fuels (here H₂), will play a major role. To achieve the targeted scale, abundant, active, and stable converter materials and to integrate them in efficient devices, i.e., artificial leaves, understanding of their interface chemistries and energetics is required.

The talk will focus on characterization and control of bulk and interfacial properties governing the functioning of solar energy materials and devices. I will introduce the requirements for successful solar water splitting devices and discuss the electronic structure of the involved functional materials – focusing on Bi-based oxides. At the example of CuBi₂O₄ as a promising p-type oxide photoabsorber, the experimental and theoretical characterization of interfacial energetics and chemistry will be discussed. Specifically, suitable contact materials to create improved performance photoelectrodes and light-driven surface modifications will be discussed in relation to the bulk and interface electronic structure of the CuBi₂O₄.^{1,2} Measurement strategies to assess the bulk and interface electronic structure, including Fermi level, as well as optical properties will be introduced. Bulk modifications by doping leading to improvement of interfacial charge carrier transfer will be shown on

n-type Mo-doped BiVO₄ photoanodes highlighting the key influence parameters routed in interface energetics and reaction kinetics.^{3,4}

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Excursion | Tuesday 5.3. | 14:00–18:00

Visit to Schloss Heiligenberg

A relaxed walk to the nearby Schloss Heiligenberg will take 30–45 minutes. At the castle, cake and coffee will be offered for refreshment. A guided tour will give a deeper insight into



the surprising history of the place. In the evening, we return to the Lufthansa-Center for dinner.

WEDNESDAY

Session 7 | *Wednesday 6.3.* | 9:00–10:20

Materials Chemistry 1 | Chair: Anke Weidenkaff

7-1 | 9:00

Discovery synthesis of inorganic functional materials in the digital age

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The need for new materials to tackle societal challenges in energy and sustainability is widely acknowledged. As demands for performance increase while resource constraints narrow available options, the vastness of composition, structure and process parameter space make the apparently simple questions of where to look for and how to then find the materials we need a grand challenge to contemporary physical science. This talk will emphasise that discovery synthesis of new inorganic materials is at the extreme forefront of this endeavour.

In this presentation, I will address the role of digital and robotic tools in discovery from the perspective of the experimental realisation of new materials with structures that differ from those in the databases [1] in a manner that has consequence for their functional performance

[2]. This will include the demonstration that it is now possible under clear assumptions to guarantee to predict the crystal structure of a material based solely on its composition [3], the role of machine learning from data in supporting decisions by experimental researchers [4; 5], and the acceleration of inorganic materials discovery with robots [6].

The role of these digital tools in a modern integrated materials discovery workflow will be presented with an example of the discovery (*i.e.*, the experimental realisation in the laboratory) of a quaternary inorganic solid that displays high lithium ion conductivity that arises from its new structure. This leads to a different perspective on how lithium ions can attain high mobility in solids [7]. Such perspectives may prove generally helpful in the design of the fast ion transporting materials that we will need across future energy technologies.

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- [2] C.M. Collins, L.M. Daniels, Q. Gibson et al., Angewandte Chemie Int Ed 60, 16457, 2021.
- [3] V.V. Gusev, D. Adamson, A. Deligkas et al., Nature 619, 68, 2023.
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Electrochemical Fluorination of Perovskite (-related) Materials – From Fundamentals to Battery Applications and what it could tell us about the Fermi Level

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An ongoing scientific challenge is to identify batteries based on ionic charge carriers other than lithium, without lowering the electrochemical voltage window. Using anions as ionic charge carriers, a similarly broad voltage window could be accessed using electrochemically stable fluoride ions as shuttle ions within Fluoride Ion Batteries (FIBs, see Figure 1a). Such FIBs were recently developed as solid state batteries consisting of conversion type electrode materials (binary metal fluorides MF_y which are transformed to the respective metal M (and vice versa) on charging/discharging of the battery). Although binary fluorides can provide high capacities, they suffer from very strong capacity fading.

In this contribution, I will give an overview about the perovskite (-related) materials which can be used as electrode materials for fluoride ion batteries. I will be shown that reversible electrochemical fluorination / defluorination can facilitate the development of cycling stable all solid state FIBs (see Figure 1b) based on Ruddlesden-Popper type compounds and that newly developed routes for the chemical defluorination of fluorinated compounds facilitate a deeper understanding of anode materials in the charged state. Finally, these results and current ongoing studies will be set in the context of changes of the Fermi Energy.

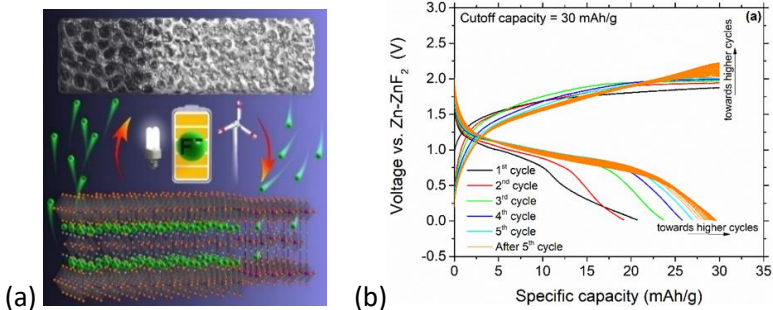


Figure 1. (a) Scheme of a FIB. (b) Cycling behavior of La_2NiO_4 against a Zn/ZnF_2 reference.

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- [3] M.A. Nowroozi, I. Mohammad, P. Molaiyan, K. Wissel, A.R. Munnangi, O. Clemens, Fluoride ion batteries – past, present, and future, *J. Mater. Chem. A* 9 (10), 5980-6012, 2021, DOI: 10.1039/d0ta11656d.
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8-1 | 10:50

Pair Distribution Function: a tool to reveal the defect structure in functional materials and nanomaterials

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The fascinating physical properties of functional crystalline materials are strictly linked to symmetry breaks at the nanoscale induced by point and extended defects, strong electron correlation and/or structural reconstruction at the surface (e.g. in nanoparticles). Therefore, a meaningful structural characterisation should encompass short-, medium-, and long-range investigations. The so-called Pair Distribution Function (PDF), that is the real space analysis of diffraction data, emerged as a powerful tool to achieve a complete and accurate structural picture at all the length scales.

After a brief introduction to the technique, some applications of PDF to materials science cases are presented. Examples will include highly defective oxides and perovskite oxides displaying symmetry breaks at the local scale. Deviation from the crystallographic average structure are introduced either decreasing the phase symmetry or relaxing the position of atoms around point defects explicitly introduced in the model. In that regard, computer-based simulations using the Density Functional Theory (DFT) approach have proven useful to gain further insight in direct combination with the experimental PDF data.

Oxygen Transport Membranes, Fermi Level Engineering, and a Grain of Sustainability

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To address climate change, CO₂ capture and utilization can help to curtail emissions and decrease atmospheric CO₂ levels. Our focus lies on plasma-assisted CO₂ and H₂ conversion to methanol as fuel (energy storage) and C1-building block for the chemical industry. To minimize recombination reactions (CO₂ & H₂O formation), mixed ionic-electronic conducting (MIEC) ceramic oxygen transport membranes (OTM) are required to control the oxygen partial pressure $p(\text{O}_2)$ in the reaction zone. This places significant demands on the materials utilized: absence of phase transitions, tolerance against CO₂, H₂ and their radical and ionic species produced in the plasma, while also maintaining balanced electronic and ionic conductivity to achieve desired oxygen permeation rates [1].

To steer all these requirements, efficient doping strategies are required. However, doping (aliovalent substitution) can induce a complex response in oxide materials, facilitating various charge compensation mechanisms. Fortunately, all charge compensation mechanisms can be described using a common energy scale, referring to the Fermi level, which can be directly measured by X-ray photoelectron spectroscopy (XPS). For MIEC-OTMs, the mixed ionic-

electronic charge compensation is crucial. Another relevant aspect is the correlation between surface exchange reactions, $p(\text{O}_2)$, and Fermi level [2]. Our model system is differently substituted/doped $\text{Ba}_2\text{In}_2\text{O}_5$. As dopants we are using $3d$ transition metals. Cr is an intriguing dopant as XPS suggests the presence of Cr^{6+} instead of anticipated Cr^{3+} , hence donor doping. A treatment in reducing conditions indicates the presence of Cr^{4+} . The Fermi level remained nearly unchanged upon doping pointing to mainly ionic charge compensation by interstitial oxygen, which is supported by the analysis of the oxygen content by neutron diffraction [3].

Given its capacity to readily utilize intermittent renewable energies, CO_2 , and green H_2 , the plasma-assisted conversion process holds promising potential for a sustainable approach. Yet, the sustainability of the process hinges on the use of membrane materials that are also sustainable. The OTMs often involve the usage of critical elements such as rare earths or cobalt, hence, it is crucial to concurrently formulate strategies for their recovery next to the materials development to achieve material circularity. As recycling processes typically involve energy and process chemicals inputs, they are not by-default sustainable. In that regard, it is crucial to prioritize monitoring the environmental impacts of the involved processes. This allows data-driven decision-making towards sustainability rather than relying on claims and perceptions [4,5].

This presentation will examine Fermi level engineering from the viewpoint of MIEC-OTMs, present initial findings, the intended application of OTMs, and a reminder of the critical shift towards a sustainable future, propelled by a novel approach to material usage and development.

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8-3 | 12:10

Near-Ambient Pressure Photoelectron Spectroscopy on Electrode/Electrolyte Interfaces: Where Fermi Level and Electrochemical Potential Meet

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In our research, we use near-ambient pressure photoelectron spectroscopy (NAP-XPS) to determine chemistry and electrical potential distribution at electrode/electrolyte interfaces. This brings challenges as we combine surface and interface science with electrochemistry in one experiment. As in classical UHV photoelectron spectroscopy, the binding energies in near-ambient pressure photoelectron spectroscopy are measured with respect to the Fermi level of the spectrometer. In electrochemistry, the driving force for the transfer of charged species from one phase to another in a redox reaction is the difference in electrochemical potential. In this presentation, we show how we bring those two views together at the contact between electrode and electrolyte in Li-ion battery model systems. We outline the relations between different potentials and present how NAP-XPS can be used to follow charge transfer reactions at the electrode/electrolyte interface, even without obtaining a signal directly from the interface. We show how we obtain information about changes in electron electrochemical potential difference over the solid/liquid interfaces by measuring the kinetic energy (KE) shifts of the electrolyte core levels [1]. And, while

indirectly, how we can follow the change in Li chemical potential of the working electrode surface at Li-ion equilibrium [2].

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- [2] I. Källquist, F. Lindgren, M.-T. Lee, A. Shavorskiy, K. Edström, H. Rensmo, L. Nyholm, J. Maibach, M. Hahlin; Probing electrochemical potential differences over the solid/liquid interface in Li-ion battery model systems; *ACS Appl. Mater. Interfaces* 13, 32989–32996, 2021.

Session 9 | Wednesday 6.3. | 14:30–16:00
JuniorFLAIR 2 | Chair: Sylvia Kunz

9-1 | 14:30

Fermi level engineering in perovskite-type oxynitride photoabsorbers

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Photoelectrocatalytic solar water splitting (SWS) is one of the evolving methods being investigated to enable the direct conversion of solar energy to hydrogen. When selecting a material for SWS, certain requirements must be met, such as an appropriate bandgap energy and band edge positions, effective charge carrier separation, strong catalytic activity, and (photo)chemical stability [1].

Among other materials, perovskite-type oxides (ABO_3) are interesting for SWS because they can be very stable in aqueous media and have high catalytic activity under UV light [2]. However, the bandgap energy of these materials is usually too high for visible light absorption. Hence, the need to reduce the bandgap by obtaining perovskite-type oxynitrides ($AB(O,N)_3$) through ammonolysis. With all the qualities of perovskite-type oxides plus a suitable bandgap, oxynitrides are appealing n-type semiconductors, being researched as photoanodes for SWS applications [3].

Replacing O^{2-} by N^{3-} in the anionic sublattice requires charge compensation, in which different mechanisms can be involved [4]. Moreover, there is currently no concept available to allow for the prediction of the dominating charge compensation mechanism in these materials. Thus, preparing bulk oxynitrides, each directed at a specific charge compensation mechanism, is a key part of this study, aiming at understanding how the different possible charge compensation mechanisms can be controlled by the Fermi level position.

Comprehending what consequences, the charge compensation mechanisms have on the photophysical properties of oxynitrides by manipulation of the Fermi level during material synthesis is crucial [5]. Consequently, the correlation between compositional variations and Fermi level position, effective bandgap, and band edges is important to determine.

This presentation aims to introduce the materials systems under research, along with initial experimental insights, and structural influencing factors on the photophysical properties.

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[3] K. Maeda et al., *MRS Bull* 36, (1), 925–31, 2011.

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9-2 | 14:45

Water adsorption on single crystal SrTiO₃ towards Fermi Level Engineering for the oxygen evolution reaction

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The electronic structure of perovskite oxides has been shown to influence the oxygen evolution reaction (OER) catalytic performance; surface properties and electronic structure of SrTiO₃ perovskites in interaction with water have already been characterized [1, 2]. However, a description of how the catalyst surface can be modified in terms of doping, substitution, or defect engineering so that a specific catalyst OER active surface phase forms and which role the Fermi Level, as well as the occupied and unoccupied states of the surface play in this transformation, remain unclear.

The OER introduces large overpotentials in water electrolysis because of its sluggish kinetics due to the four-electron transfer process. By heterovalent substitution in oxide electroceramics (doping), different compensation mechanisms (electronic, ionic, valence changes...) can be enabled.

The *collaborative research center FLAIR* is working on being able to predict and apply these different compensation mechanisms. We propose that the Fermi Level can be used as a universal descriptor for

these compensation mechanisms and will be integral for creating efficient and stable perovskite OER catalysts in the future on the principles of Fermi Level engineering [3].

As described by Ede and Luo [4], it is known that doping, by changing the electronic structure, can influence the OER catalytic performance since it can change the binding energy of OER intermediates, such as oxygen, hydroxide, and oxyhydroxide species. Oxygen vacancies are also known to influence the water adsorption behavior of perovskites and to improve the dissociation of water on the surface of perovskites [5]. The Ti^{3+} states created to compensate for these vacancies should be visible in the valence band around 0.3 eV to 1.3 eV.

For systematically checking the influence of electronic structure changes due to doping on single crystalline $SrTiO_3$ we are looking at (100), (110) and (111) oriented single crystalline samples without doping for a pristine comparison, 0.05 wt.% and 0.1 wt.% Nb doping for low doping concentrations and 0.7 wt.% Nb doping for high doping concentrations (all single crystals bought from MaTeck).

After an etching procedure to receive atomically flat surfaces, a chemical cleaning is performed, and the single crystals are heated in oxygen in our integrated vacuum cluster tool system DAISY FUN, to prepare atomically clean single crystalline $SrTiO_3$ surfaces. On these surfaces water adsorption experiments are performed at room temperature and with liquid nitrogen cooling (with and without UV light irradiation) in order to connect the electronic structure with its temperature- and photo-activated water adsorption behavior. AFM, LEED, XPS and UPS measurements are performed to check the surface structure and composition before and after water adsorption. Additionally (Photo)electrochemical measurements are performed on

the single crystals in alkaline conditions. First results are going to be presented.

[1] Solokha et al., J. Phys. Chem. C, 123, 17232–17238, 2019.

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9-3 | 15:00

Machine Learning Interatomic Potential for Barium Titanate: Applications to Phase Transitions, Pressure Effects, and Grain Boundaries

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Barium titanate (BaTiO_3), a prototypical perovskite oxide, exhibits complex ferroelectric phase transitions from a high-temperature cubic paraelectric phase transforms into a series of lower-temperature phases (Tetragonal \rightarrow Orthorhombic \rightarrow Rhombohedral). These transitions are characterized by order-disorder transitions. While ab-initio molecular dynamics can model finite-temperature properties, computational demands limit simulations to small systems and short timescales. Classical molecular dynamics offers efficiency but often sacrifices the accuracy of first-principles methods. To address these challenges, we introduce a machine learning interatomic potential (MLIP) for BaTiO_3 built upon the Atomic Cluster Expansion (ACE) framework and trained with density functional theory (DFT) data. This potential replicates DFT accuracy while enabling simulations across significantly larger time and length

scales. Our research uses this potential to study the temperature-driven cubic-to-rhombohedral phase transition in BTO and how pressure affects the transition temperature. Additionally, we demonstrate the potential's ability to model BTO grain boundaries and domain wall structures. We compare the performance of our BTO machine learning potential to a traditional shell-type model for different grain boundary structures in BTO.

9-4 | 15:15

Electro-chemo coupled phase field modeling of the equilibrium space charge layer formation in Fe-doped SrTiO₃

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Owing to the segregation of point defects in the grain boundary region, the space charge layer forms and the grain growth kinetics are consequently altered. In order to reproduce the formation of space charge layer at equilibrium state, sharp interface model is developed by De Souza [1] and the space charge layer potentials are quantitatively predicted. Aiming to avoid tracking the grain boundary position and simulate more complex grain growth processes, in the present work, we have developed an electro-chemo coupled phase field model linking to the thermodynamic model described in De Souza's paper [1]. Then, the capabilities of this model are benchmarked via simulating Mott-Schottky and Gouy-Chapman space charge layers in the bicrystal of Fe-doped SrTiO₃. For different segregation energies of oxygen vacancy and iron point defect between bulk phase and core region, the space charge layer potentials obtained by phase field simulation agree well with sharp interface calculations. Furthermore, the concentration profiles of

different point defects and electrostatic potential profiles are extracted from phase field simulations, which have a nice agreement with sharp interface predictions.

[1] De Souza R A. The formation of equilibrium space-charge zones at grain boundaries in the perovskite oxide SrTiO₃. Physical Chemistry Chemical Physics 11 (43), 9939-9969, 2009.

9-5 | 15:30

Mapping the Space Charge Region in BaTiO₃ and SrTiO₃ using 4-Dimensional Scanning Transmission Electron Microscopy

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Ceramic capacitors are passive electronic components designed to store and release electrical energy through an electric field [1]. Polycrystalline barium titanate (BaTiO₃) and strontium titanate (SrTiO₃) have been widely employed in ceramic capacitors due to their reliable dielectric properties, compact size, and cost-effectiveness [2]. However, this material experiences degradation, such as increased leakage current, as a result of diminishing resistance under elevated temperatures and voltage stress.

According to the ionic de-mixing model, the primary cause of this degradation is the migration of oxygen vacancies, which move toward grain boundaries and eventually reach the cathode [3].

The migration of oxygen vacancies can be effectively altered by doping with elements such as Fe and Mn. This doping modifies the Fermi level and the space charge region (SCR) at grain boundaries. The SCR is the result of an accumulation or depletion of oxygen vacancies and cations around grain boundaries, limiting their migration and preventing degradation. However, this general description lacks validation of the details such as the influence of grain boundary character on the SCR due to limited microscopic observations of grain boundaries and SCR in ceramic capacitors, making it challenging to further develop the theory.

In this study, we employ 4-dimensional scanning transmission electron microscopy (4D-STEM) [4] in combination with electron precession to map electric fields at grain boundaries in Fe-doped BaTiO₃ and SrTiO₃. Unlike conventional differential phase contrast (DPC) analysis, electric field mapping by 4D-STEM reduces diffraction and channeling artifacts thus enabling accurate measurement of electric field and charge density at the grain boundary. Combining it with an in-situ biasing TEM setup, we can visualize SCRs under different biasing conditions at various temperatures. Through our presentation, we aim to showcase our methodological developments and observations of SCRs in BaTiO₃ and SrTiO₃. These findings promise to significantly advance the fundamental scientific understanding of ceramic capacitor performance and illuminate the degradation mechanisms under high voltage stress.

[1] K. Hong, T.H. Lee, J.M. Suh, S.-H. Yoon, and H.W. Jang, Perspectives and challenges in multilayer ceramic capacitors for next generation electronics, *Journal of Materials Chemistry C* 7 (32), 9782–9802, 2019.

- [2] M.M. Vijatović, J.D. Bobić, and B.D. Stojanović, History and challenges of barium titanate: Part II, *Science of Sintering* 40.3, 235-244, 2008.
- [3] R. Giesecke, R. Hertwig, T.J.M. Bayer, C.A. Randall, and A. Klein, Modification of the Schottky barrier height at the RuO₂ cathode during resistance degradation of Fe-doped SrTiO₃, *Journal of the American Ceramic Society* 100 (10), 4590–4601, 2017.
- [4] S. Kang et al., Direct observation of quadrupolar strain fields forming a shear band in metallic glasses, *Advanced Materials* 35 (25), 2212086, 2023.

9-6 | 15:45

Accelerated Cation Diffusion along Grain Boundaries in Acceptor-doped Strontium Titanate

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The basic picture of the electrical properties of grain boundaries in acceptor-doped titanate perovskites is well established: The boundaries bear a positive charge, arising from segregated oxygen vacancies, that is accompanied by adjacent negative space-charge zones. Here point defects with a positive relative charge (oxygen vacancies, electron holes) are depleted and point defects with a relative negative charge (acceptor dopants, electrons, cation vacancies) are accumulated. The quantity that describes the degree to which point defects are depleted or accumulated within the space-charge layers is the space-charge potential. The main objectives of this work are to characterize the space-charge potential at the grain boundaries and understand the measured behaviour of the space-charge potential as a function of temperature, oxygen partial pressure and thermal treatment in terms of Fermi levels and point-defect formation in the bulk and at the grain boundaries.

In this study, thin films of BaZrO₃ were deposited on SrTiO₃ to probe the diffusion of Ba and Zr into polycrystalline, acceptor-doped SrTiO₃ ceramics. Diffusion experiments were performed at various temperatures in air as a function of diffusion time t . Diffusion profiles were measured with Secondary Ion Mass Spectrometry. The resulting diffusion profiles showed two features: the first feature being attributed to slow diffusion in the bulk and the second feature to fast diffusion along grain boundaries. Thorough analysis of this data yielded the bulk diffusion coefficient D_b as well as the grain-boundary diffusion product $sw_{gb}D_{gb}$, from which, in the future work, the space-charge potential will be extracted.

Session 10 | Wednesday 6.3. | 16:40–18:15
Wrap-up and Outlook | Chair: Andreas Klein

10-1 | 16:40

Computational Prediction of the Fermi Level in Electroceramics

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The functional properties of electroceramics oxides are directly depending on a number of factors, including the presence of dopants, impurities, dislocations, grain boundaries, processing history and so on. Thus, a quantitative description of structural and electronic properties of defects, their interactions and related compensation mechanisms which determine the Fermi level is essential for a future materials design. Computational modelling of

point defect equilibria has become a standard tool in recent years. However, predicted defect equilibria and charge transition levels are very often not in line with experimental results.

In this presentation, I will discuss examples of defect calculations, the prediction Fermi levels and their relation to experimental findings. The focus will be on the role of processing conditions and polymorphism [1], interactions of oxygen vacancies and dopants [2], the influence of point defects on phase diagrams [3] and the interaction with 1-dim. lattice defects [4].

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[4] M. Sadowski et al., Chemistry of Materials 35, 584-594, 2022

11-2 | 17:20

Feedback, Discussion, Outlook

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