# SYEM 1: Emerging Materials for Renewable Energy Conversion

Time: Wednesday 9:30–12:15 Location: H 0105

**Invited Talk** SYEM 1.1 Wed 9:30 H 0105

**Non-critical Materials Production for a Green Energy Transition** — •Anke Weidenkaff, Wenjie Xie, and Marc Wiedenmeyer — Technische Universität Darmstadt

The defossilisation of the energy sector requires a green infrastructure for efficient renewable energy converters.

The new infrastructure cannot be based on critical materials. Therefore, the transformation to a future fossil free green circular economy will be based on sustainable materials production processes and ecologic innovations.

The development of renewable materials for renewable energy converters requires the development of an affordable but sustainable large-scale production from secondary raw materials. The decision making for future resilient energy systems has to be based on fair, ecological and economical aspects and data from performance criteria defined by a holistic life cycle assessment.

In this lecture a recycling / production of materials with a programmable lifetime and self regeneration will be introduced as a suitable approach.

The design of circular high performance materials uses theoretical predictions and the criticality analysis of applied elements to improve the cycle life of future energy converters such as thermoelectric generators and refrigerators, batteries, electrolysers, fuel cells, plasmalysers, hydrides and solar watersplitting cells.

**Invited Talk** SYEM 1.2 Wed 10:00 H 0105

**Strategies for the morphological design of photoactive oxynitride particles and electrodes for solar water-splitting.** — •Simone Pokrant — Chemistry and Physics of Materials, Paris-Lodron University Salzburg, Austria

More than 50 years after the first demonstration of photocatalytic water-splitting by Fujishima and Honda in 1972, the exploitation of photocatalytic and photoelectrochemical water-splitting for solar fuel production is still hindered by an unfavorable device-efficiency-versus-cost ratio. For these applications high active surface areas and favorable charge transport properties are key features to enhance device performance. Acceptable charge transport properties are usually obtained in defect free structures such as single crystals, where the surface area is small in comparison to agglomerates of porous nanoparticles. Nanoparticles and nanoparticle agglomerates, however, suffer from reduced charge extraction and, when deposited onto electrodes for photoelectrochemical applications, from charge transport limitations to the back contact because of multiple grain and particle boundaries. Lately, the careful design of single-crystalline particles with well-defined facets and decorated with cocatalysts has served as a successful concept to achieve high efficiencies in the case of the UV light sensitive model system SrTiO3. In this contribution, perovskite-related oxynitrides will be introduced as a promising visible light absorbing photocatalytically active material class. It will be shown how the conversion of oxides to oxynitrides via thermal ammonolysis enables particle design for improved photocatalytic and photoelectrochemical performance.

**Invited Talk** SYEM 1.3 Wed 10:30 H 0105

**Computational workflows for an accelerated design of novel materials and interfaces** — •Ivano Eligio Castelli — Department of Energy Conversion and Storage

The development of automated computational tools is required to accelerate the discovery of new functional materials, to speed up the transition to a sustainable future. Here, I address this topic by designing new electrodes with controlled interfaces for different applications which accelerate the transition to a sustainable future. These workflows are implemented in the framework of Density Functional Theory (DFT), using MyQueue and the Atomistic Simulation Environment (ASE). I Starting from our recent work on a fully autonomous workflow, which identifies materials to be used as intercalation electrodes in batteries, based on thermodynamic and kinetic descriptors like adsorption energies and diffusion barriers, I will describe a new modular approach to estimate electronic and ionic mobility in energy materials useful for a variety of applications, from batteries and fuel cells and solar energy conversion and storage. A substantial acceleration for the calculations of the kinetic properties has been obtained using a surrogate model to identify the transition states, which can further reduce the computational cost to at least one order of magnitude. I will also describe my vision for autonomous computational workflows, namely the creation of workflows for interface and their integration with experimental workflows.

**30 min. break**

**Invited Talk** SYEM 1.4 Wed 11:30 H 0105

**Autonomous composition control of emerging nitride materials for solar energy conversion** — •Andriy Zakutayev — National Renewable Energy Laboratory, Golden CO, USA

New photoabsorber materials, including nitrides, are desired for solar energy conversion into chemical feedstocks such as hydrogen and liquid fuels. However, experimental realization of computationally predicted absorber candidates is challenging, and synthesis optimization to achieve theoretical properties is time-consuming. In this talk, I will show how experimental synthesis of epitaxial thin films of emerging ZnTiN2 photoabsorber [1] can be aided by autonomous control of its chemical composition [2]. Bayesian algorithms fed by optical plasma emission spectroscopy are used to control Zn and Ti precursor fluxes and other sputter deposition parameters to achieve the desired ZnTiN2 composition for different deposition conditions. High-quality (001) oriented ZnTiN2 wurtzite thin films on sapphire substrates are achieved with atomically flat surfaces, suitable for epitaxial integration with III-N and II-O wurtzite semiconductors into photoelectrochemical energy conversion devices. Together, these results illustrate the promise of autonomous control methods for accelerated synthesis of emerging materials for renewable energy conversion. Accelerated measurements of electrochemical impedance spectroscopy using autonomous characterization methods will be also discussed. [1] JACS 144, 13673 (2022) [2] APL Mater. 11, 071119 (2023)

**Invited Talk** SYEM 1.5 Wed 11:45 H 0105

**Understanding and tailoring the catalytic activity of spinel and perovskite surfaces from first principles calculations** — •Rossitza Pentcheva — University of Duisburg-Essen, Department of Physics, Germany

The optimization of catalysts for chemical energy conversion such as the (photo-) electrocatalytic water splitting requires mechanistic understanding at the atomic level. Based on density functional theory (DFT) calculations with a Hubbard $U$ term, we focus on the oxygen evolution reaction (OER) at iron, cobalt and nickel containing spinels [1-3] vs. perovskites [4-5]. This allows us to disentangle the role of structural motifs, crystallographic orientation, termination and dopants. Analysis of the underlying electronic and magnetic properties reveals dynamic variation of oxidation state of surface cations during OER with marked differences in the degree of localization in spinels and perovskites. Octahedral Co at the (001) surface emerges as a potential active site with the lowest overpotentials. Finally, we assess the effect surface transformation into an oxyhydroxide layer at $LaNiO_3$ and identify important distinctions for different surface facets that eventually control the OER activity [5]. Funding by the German Research Foundation within CRC TRR247 and computational time at the Leibniz Rechenzentrum and the supercomputer MagnitUDE at UDE are gratefully acknowledged. [1] ACS Catal. 8, 11773 (2018); [2] ACS Catal. 11, 5601, (2021); [3] Adv. Funct. Mater. 33, 2210945 (2023); [4] Chem. Eur. J. 27, 17145 (2021); [5] A. Füngerlings et al, Nat. Commun, in press.

**Invited Talk** SYEM 1.6 Wed 12:00 H 0105

**Mastering Compositional Complexity in High Entropy Materials for Energy Applications - Towards Accelerated Materials Discovery by Integration of High-throughput Experimentation, Simulation, and Materials Informatics** — •Alfred Ludwig — Ruhr-Universität Bochum

Discovery of new materials is a key challenge in materials science. New materials for a sustainable energy system are necessary. Compositionally complex materials, ("high entropy materials"), offer a vast multi-dimensional search space, which provides opportunities for discovering new materials. However, efficient methods for the exploration and exploitation of this search space are necessary. Integration of high-throughput thin-film combinatorial materials science methods with

simulation and materials informatics is an effective means to produce large datasets on new materials, which enables mastering of the search space. Theoretical predictions from high-throughput computations are combined with production of large, consistent and complete experimental datasets, which are used for materials informatics. Thin-film materials libraries are fabricated by combinatorial sputter deposition and analysed by high-throughput characterization. The talk discusses examples of combinatorial discoveries and the targeted development of new materials for electrocatalysis where compositional complexity offers a new design principle. Furthermore, applications of materials informatics to accelerate and improve the materials discovery process are presented.