Data and metadata schema for high-throughput characterization of energy materials

Supervisors

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Number of Candidates: 1

Backgrounds of Candidates

The ideal candidate has an interest in solid state physics and experience coding in Python or MatLab. Some laboratory experience with characterization techniques, such as X-ray diffraction, spectrophotometry, electrical conductivity measurements, or thin film growth by pulsed laser deposition, is advantageous. A genuine interest in combinatorial materials science, high-throughput screening of spatially addressable material libraries or data-driven science is also beneficial.

Project Descriptions

The objective of the project is to substantially accelerate the experimental determination of the key physical properties of novel energy materials that have potential application in top cells of tandem photovoltaic (PV) structures or in photoelectrochemical (PEC) water splitting cells. The project also aims to process the associated material properties in a FAIR data schema and to enter all relevant data and metadata into the UiO eLabNext electronic lab notebook (ELN). The proposal addresses two subjects relevant for UiO:Energy and Environment: the primary research area "Energy Systems, Materials, and Models," and the overarching cross-cutting theme of "Digitization."

In this project, we will realize a continuous composition spread material library by combinatorial pulsed laser deposition [1] in MiNaLab. A particularly promising, albeit not yet thoroughly investigated, ternary material system that has emerged is $(Ti_xFe_{1-x})_2O_3$, which adopts a rhombohedral corundum crystal structure. The fundamental bandgap of the binary materials is approximately 2.2eV and 0.1eV for α-Fe_2O_3 and α-Ti_2O_3, respectively [1]. Furthermore, the averaged bond lengths of 2.03 Å and 2.05 Å (cf. Fig. 1) are very similar, suggesting that miscibility is expected across the entire phase diagram [2]. This renders the α-$(Ti_xFe_{1-x})_2O_3$ ternary system an ideal candidate for high-throughput characterization of material properties relevant for photovoltaic and photocatalytic applications. This approach relies on methods with sufficiently high spatial resolution that allow for systematic mapping of sample positions and systematic screening of properties as a function of chemical composition. In MiNaLab, the chemical composition and structural information of materials can be determined with high spatial resolution. This determination is made possible by automated mapping routines. To date, the measurement of optical and electrical properties has been possible only through a time-consuming one-by-one sampling approach, despite the technical feasibility of a mapping method. The scope of the project is therefore twofold: One component of the project entails the development of a control software that facilitates the user-friendly implementation of the mapping capabilities of the spectrophotometer and the electrical probe station. The software will further structure and save the experimental data in a FAIR[1] way that enables AI- and machine learning assisted analysis. The necessary data schemas will be

[1] **F**indable, **A**ccessible, **I**nteroperable, **R**eusable

developed within the project. If such schemas are available from other sources (e.g. the FAIRmat initiative) they will be considered and potentially adopted to our needs. This will enable other scientists to comprehend the data and, in principle, redo the measurements identically. The schema employed for the data structure will undergo parsing into the ELN ELabNext using a corresponding template (developed as part of the project), wherein it is structured and stored in conjunction with the results of the chemical and structural analysis.

In this project, the summer scholar will investigate the continuous composition spread energy material library using spatially resolving methods to determine key functional properties in relation to the chemical composition. This combinatorial materials science approach allows the scholar to acquire a comparatively large dataset with much higher chemical resolution than traditional one-by-one investigations of ternary alloys. This will enable the student to work with and analyze a large, high-quality dataset obtained by state-of-the-art, high-throughput characterization of a single sample (a single, spatially addressable material library). The scholar will receive training in energy materials, their characterization and their potential applications, as well as the structured digitization of experimental datasets (FAIR data structure and digitization of all relevant data and metadata), the possibilities and limitations of the available high-throughput methods at MiNaLab, and programming software that enables existing hardware to map data in an automated, high-throughput fashion. Additionally, the scholar will identify compositions of particular interest for photovoltaic (PV) and photoelectrochemical (PEC) applications that will be investigated in more detail within lab-scale demonstrator devices in the SOLARIS project.

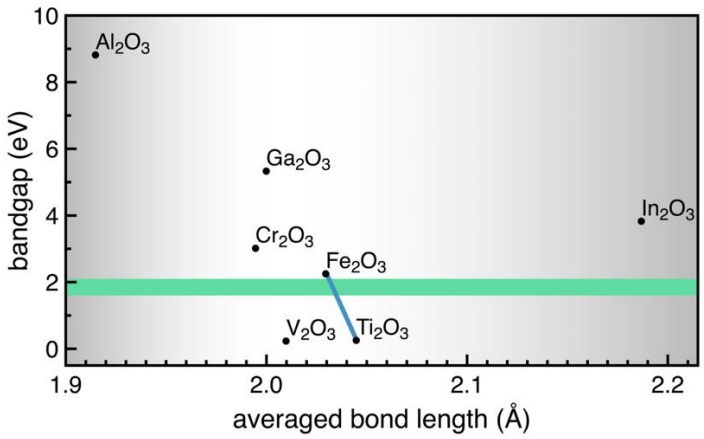


Figure 1. Fundamental bandgap of corundum-structured group-III and transition metal sesquioxides as a function of the averaged bond length. The green box indicates the bandgap energy range of interest for PEC and Tandem PV applications. The blue line highlights the expected variation of bandgap and averaged bond length for the α-$(Ti,Fe)_2O_3$ material library.

The project should run at any time between April and September of 2026.

References

[1] H. von Wenckstern, M. Andreassen, K.G. Both, Fundamentals of pulsed laser deposition, advanced developments and implementation of combinatorial material synthesis, and its application to the growth of Ga2O3 and related alloys, Editor: Roberto Fornari, Comprehensive Semiconductor Science and Technology (Second Edition), Elsevier, 2025, Pages 225-266, ISBN 9780323958196, https://doi.org/10.1016/B978-0-323-96027-4.00042-5.

[2] Fujita, S. & Kaneko, K. Epitaxial growth of corundum-structured wide band gap III-oxide semiconductor thin films. *Journal of Crystal Growth* **401**, 588–592 (2014).