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Quantification of Dynamic Structural Disorders in Energy Conversion Materials

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Defects and structural disorders are well recognized as crucial for the energy conversion process. However, the precise description of the types and concentrations of defects is an intriguing and complex challenge, requesting the combination of various advanced experimental in situ and post mortem methods such as laboratory- and synchrotron-based X-ray diffraction, neutron diffraction, X-ray photoelectron spectroscopy, and electrical transport properties as well as theoretical modeling and simulation techniques. In particular, the changes of the defects and disorder happen in most energy conversion processes affected by environmental factors such as temperature changes or light excitation. Four types of materials are currently in the focus of our research where the defect structure and dynamics are to be understood in detail: i) the change in the occupation of the ideally empty structural site in thermoelectric half-Heusler materials leading to disorder and intrinsic doping effects by the creation of in-gap states in the band structure[1,2], ii) the transport of oxygen ions via (disordered) oxygen vacancies and electrons in oxygen transport membrane materials for the plasma-assisted CO2 conversion[3,4], iii) perovskite-type oxynitrides for solar water splitting containing Ta4+ or Ta5+ on the B-site showing presence or absence of O/N ordering depending on the investigated length scale[5,6], and finally iv) the role of defects on optical properties of perovskite-type halides for photovoltaics[7,8].
Basically, the dynamics of the defects and disorder are expected to play a crucial role for the efficiency and lifetime of an energy conversion material. Except for photovoltaic and other photo-induced converters, such dynamic effects are studied relatively seldom[9]. In addition to the methods mentioned above, time-resolved measurements, e.g., by neutron spectroscopic methods are necessary to get experimental access to the ongoing changes in a material during energy conversion. An extended understanding of the dynamic phenomena is needed in order to enable a conceptional implementation into future material design. Accordingly, this will allow a longer lifetime of the material in a specific energy conversion process helping also to reduce the demand for material resources.

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Primary authors: Dr WIDENMEYER, Marc (Technische Universität Darmstadt); Dr XIE, Wenjie (Technische Universität Darmstadt); Dr YAN, Ruijuan (Technische Universität Darmstadt); Dr YOON, Songhak (Fraunhofer Research Institution for Materials Recycling and Resource Strategies IWKS); Prof. WEIDENKAFF, Anke (Technische Universität Darmstadt)

Presenter: Dr WIDENMEYER, Marc (Technische Universität Darmstadt)

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