TUT 4: Strategic elements and sustainability (joint session MA/TUT)

Our appetite for resources is insatiable. The path to a climate-neutral society and economy requires the increasingly intensive use of strategy metals such as lithium, cobalt, nickel, but also the group of rare earth elements. This major transformation is not possible without the sustainable use of these so-called critical elements along the entire value chain. In the Tutorial "Strategic elements and sustainability", we have four eminent speakers looking in this context at new developments in batteries, catalysis, thermoelectrics and magnetism.

Organizers: Oliver Gutfleisch (TU Darmstadt) and Heiko Wende (U. Duisburg-Essen).

Time: Sunday 16:00–18:00 Location: HSZ 04

Invited Talk TUT 4.1 Sun 16:00 HSZ 04

Making better batteries? – From Li-ion to Na-ion batteries — •Philipp Adelhelm — Humboldt-University Berlin, Berlin, Germany — Helmholtz-Zentrum Berlin, Berlin, Germany

The shift to electromobility is one of the most important transformations currently taking place in our society. This is associated with a sharp increase in battery production, which on the one hand opens up new opportunities, but on the other hand also has a massive impact on raw material supply and supply chains. In addition, new large markets are emerging, such as stationary energy supply or mobile robotics. Lithium-ion batteries are currently the most attractive technology for this. However, due to the large demand for batteries and the different application scenarios, other technologies are also being pursued. Sodium ion batteries can be produced on the same production lines as lithium ion batteries and are therefore considered a "drop-in" technology. The aim here is to replace not only costly lithium but also other expensive elements such as nickel or copper. Work is therefore being done worldwide on a cell chemistry for sodium ion batteries that works almost as well as lithium ion technology, but at the same time is cheaper and more readily available, or has other specific advantages. The tutorial gives an introduction to sodium ion technology. The motivation and state-of-the art are explained in more detail and material aspects are discussed. In particular, the question is addressed which electrode materials are promising for sodium ion batteries, what is needed to achieve further progress and what actually happens when lithium ions are replaced by sodium ions in a battery.

Invited Talk TUT 4.2 Sun 16:30 HSZ 04

Sustainable Thermoelectric Materials Predicted by Data Mining and Machine Learning — •Kornelius Nielsch — Leibniz Institute of Solid States and Materials Research, Dresden, Germany — Institute of Materials Research at TU Dresden, Germany — Institute of Applied Physcis at TU Dresden, Germany

Generating electricity from temperature differences has proven itself in space. Thanks to this technology, the Voyager probes launched in 1977 are still sending signals today. In the meantime, the car industry and ship producers have become interested in thermoelectrics. The combustion of fossil fuels produces exhaust gas that is up to 1300 °C hot. Modern thermoelectric materials are continuously expanding the fields of thermoelectric applications. The experimental search for new thermoelectric materials remains largely restricted to a limited number of successful chemical and structural families, such as chalcogenides, skutterudites and zintl phases. In principle, computational tools such as density functional theory (DFT) offer the possibility of directing experimental synthesis efforts towards very different chemical structures. In practice, however, predicting thermoelectric properties based on first principles remains a difficult endeavour, and experimental researchers do not usually use computations directly to drive their own synthesis efforts. Strategies to bridge this practical gap between experimental requirements and computational tools will be discuss und presented in this tutorial talk. Ref: Energy Environ. Sci. 14, 3559 (2021) and Advanced Theory and Simulations 5, 2200351 (2022)

Invited Talk TUT 4.3 Sun 17:00 HSZ 04

Design strategies for electrocatalysts – an electrochemist's perspective — •Kristina Tschulik — Ruhr-Universität Bochum, Faculty for Chemistry and Biochemistry, Chair for Electrochemistry and Nanoscale Materials — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf

The aim to produce highly active, selective, and long-lived electrocatalysts by design drives major research efforts toward gaining fundamental understanding of the relationship between material properties and their catalytic performance. Surface characterization tools enable to assess atomic scale information on the complexity of electrocatalyst materials. Advancing electrochemical methodologies to adequately characterize such systems was less of a research focus point. In this tutorials, we shed light on the ability to gain fundamental insights into electrocatalysis and establish design strategies based on these. Concepts on how to improve mass transport, e.g. by exploiting magnetic fields are highlighted in this respect. Particular attention is paid to deriving design strategies for nanoelectrocatalysts, which is often impeded, as structural and physical material properties are buried in electrochemical data of whole electrodes. Thus, a second major approach focuses on overcoming this difference in the considered level of complexity by methods of single-entity electrochemistry. The gained understanding of intrinsic catalyst performance will ultimately allow us to advance design concepts to transforming "pre-catalysts" in the forseeable future.

Invited Talk TUT 4.4 Sun 17:30 HSZ 04

Green magnetic materials for efficient energy, transport and cooling applications — •Oliver Gutfleisch — TU Darmstadt, Material Science, Functional Materials

High performance hard and soft magnets are key components of energy-related technologies, such as direct drive wind turbines and e-mobility. They are also important in robotics and automatization, sensors, actuators, and information technology. The magnetocaloric effect (MCE) is the key for new and disruptive solid state-based refrigeration. Magnetic hysteresis and its inherent energy product characterise the performance of all magnetic materials. In the 60th position of the periodic table of elements is neodymium - an element that belongs to the rare earth-lanthanides and essential for the above applications. Basic material requirements, figure of merits, demand and supply, criticality of strategic elements and their recycling are explained for both permanent magnets and magnetocalorics referring to the benchmark materials NdFeB and LaFeSi. Every battery needs a magnet. 95% of electric vehicles utilize rare earth magnet-based drive motors, the quantities required global will grow from 5.000 t in 2019 to about 40.000 - 70.000 t per anno in 2030. The material history of neodymium is exciting and complex; monopolistic mining in China under ruinous conditions is just as problematic as our dependence on it. How "green" are the metals for renewable technologies? Who pays which price for it, and when?