TUT 4: Tutorial: Photocatalysis (HL/O)

Time: Sunday 16:00–18:15 Location: HSZ 403

Tutorial TUT 4.1 Sun 16:00 HSZ 403

An Introduction to Rechargeable Battery Technology and Current Research Trends — •Bryan McCloskey — Department of Chemical and Biomolecular Engineering, UC, Berkeley, CA, USA — Energy Storage and Distributed Resources Division, LBNL, Berkeley, CA, USA

From electric and plug-in hybrid vehicles gaining a foothold in the automotive market to the 787 airline and Galaxy Note 7 battery fires, battery technology has, for better or worse, found itself in the popular spotlight in recent years. This spotlight is likely to shine brighter in the future, as improvements in both capability and size of portable electronic devices will make batteries and battery research increasingly important in the coming decade. Nevertheless, the 787 and Galaxy Note 7 incidents highlight an interesting dichotomy in battery research: although decades of development have allowed rechargeable batteries to be used in advanced applications, our understanding of how to design a safe, high energy density, low cost rechargeable battery still needs to be improved. This talk will initially give a general introduction to battery technology, including Li-ion batteries, focusing on their chemistry and applications. The second part of the talk will outline research directions associated with improving rechargeable batteries, with a specific emphasis on research activities for advanced materials development, including solid-state batteries and the so-called *beyond Li-ion* chemistries (Li-S, Li-air (O2), and Mg-ion batteries).

Tutorial TUT 4.2 Sun 16:40 HSZ 403

Theory and Simulations for All-Solid State Batteries — •Christoph Scheurer — Theoretische Chemie, TU München, Lichtenbergstr. 4, 85748 Garching, Germany

The concept of an All-Solid State Battery (SSB) has recently attracted substantial interest for its potential advantages over conventional liquid electrolyte-based batteries, which are slowly approaching their fundamental limitations. The SSB is often considered inherently safe due to the intrinsic separator function of solid electrolytes, as well as longterm stable, being based exclusively on solid inorganic or polymer electrolytes and electrodes and thus avoiding the use of potentially volatile and flammable organic solvents. The lack of a liquid electrolyte, on the other hand, also poses several challenges like e.g. interfacial resistances or mechanical stress and contact loss at solid-solid interfaces, which need to be fully understood and overcome for a functional, competitive SSB.

In this tutorial we will discuss key topics within the theory of superionic and mixed ionic-electronic conductors to understand the requirements for solid state electrolytes, electrode materials and their interplay. Traditional electrochemical concepts will be connected to recent atomistic simulations employing density functional theory (DFT) electronic structure, force-field based molecular dynamics (MD) and Monte-Carlo (MC), as well as coarse-grained kinetic Monte-Carlo (kMC) computations.

Coffee Break

Tutorial TUT 4.3 Sun 17:35 HSZ 403

Solid State Ionics - Mechanisms and Experimental Methods in Battery Research — •Ruediger-A. Eichel — Forschungszentrum Juelich, Institut fuer Energie- und Klimaforschung — RWTH Aachen, Institut fuer Physikalische Chemie

Solid-State Batteries promise safe, long-lived, high volumetric energy density and easily miniaturized (as thin films) devices for energy storage. However, because high currents generally only cross solid-solid interfaces at high transition resistances, current solid-state batteries mainly are limited to low-power densities.

In this contribution, the underlying principles of Solid-State Ionics, i.e. the foundations of charge transport and transfer in the 'bulk' and accross boundaries, are outlined together with an introduction of the most prominent experimental techniques for characterization of these phenomena and mechanisms. Furthermore, recent examples of application in the field of Solid-State Batteries are outlined.