Live session of seminar series **Focus Materialchemie** – Wednesday, **12.04.2023** 16:00 **@ Seminarraum Lehar 01** (TU-Wien, Getreidemarkt 9, BC, OG. 01, room A46) – **ZOOM** (ID: 983 0066 2349)

Modeling Electrochemical Systems by Density Functional Theory - Batteries and Beyond

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Computational studies have become an indispensable part of todays material science. In particular, density functional theory based methods have evolved to an essential tool for understanding and predicting material properties. As a consequence, the field of electrochemistry, including batteries with their inherent system complexity, has also largely profited from theoretical insights gained via atomistic simulations [1].

In this talk, after a general introduction to current battery research, selected anode and cathode materials for post–Li–ion batteries will be discussed. An in depth study of the alkali metal storage in hard carbon, as well as theoretical insights in the intercalation mechanism in Fe–doped CeO_2 will be presented as exemplary cases on the anode side. Weberite-type metal fluorides are discussed as potential cathode materials for Na-ion batteries, focusing on structural and kinetic aspects of these compounds. Finally, the storage mechanism of aqueous Zn batteries with a V_2O_5 cathode is presented as use case for grand canonical approaches applying the computational hydrogen electrode [1].

The talk will conclude by giving a perspective on negative emission technologies, discussing the (photo-electrochemical) reduction of CO_2 on a Ce metal catalyst.

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1. H. Euchner and A. Groß, Atomistic modeling of Li- and post-Li ion batteries, Phys. Rev. Materials 6, 040302 (2022).