MM 46: Materials for Energy Storage and Conversion - Electronic Properties

Time: Wednesday 17:15–18:30 Location: IFW D

MM 46.1 Wed 17:15 IFW D

Oxygen Vacancy Formation and Diffusion in Oxide Electrode Materials for High-Temperature Electrolysis — •Hanna Tuerk, Karsten Reuter, and Christoph Scheurer — Technical University of Munich

In a sustainable energy system, the intermittency of green electricity needs to be addressed. One possible solution to stabilize the grid are solid-oxide electrolyzer cells (SOECs), which are able to store excess electric energy into hydrogen on demand [1]. While such high-temperature SOECs are in principle well adapted to intermittent operation with frequent start-ups and shut-downs, cell performance and lifetime of existing SOECs is severely limited by anode degradation [2].

This degradation goes hand in hand with the oxygen evolution reaction (OER) taking place at the triple-phase boundary between the electrode, the electrolyte and the gas phase. In order to shed light on this degradation mechanism, oxygen vacancy formation and defect mobility at the interface of the standard electrolyte yttria-stabilized zirconia (YSZ) and the typical electrode material strontium doped lanthanum manganite (LSM) are investigated theoretically. The structural complexity of the active catalyst region mandates the use of an efficient polarizable force field, which is able to provide insight into the atomistic processes at the higly disordered interface.

[1] S. Foit *et al.*, Angew. Chem. Int. Ed. 56, 5402 (2017).
[2] M. S. Sohal *et al.*, J. Fuel Cell Sci. Tech. 9, 011017 (2012).

MM 46.2 Wed 17:30 IFW D

An ultrafast graphite oxide-graphite capacitor enabled by potassium-based ether electrolyte — •Chenglin Zhang, Long Liu, Yuhan Wu, and Yong Lei — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Graphite oxide-graphite hybrid capacitor which can offer energy between batteries and supercapacitors while in principle offering supercapacitor-like power and cyclability values was proposed as a supplementary to batteries. This prototype not only explores cheaper potassium to replace lithium to reduce costs but also employ mature commercial graphite as the negative electrode and its derivative as the positive electrode to further reduce costs and improve the prospect of commercialization. The potassium-based ether electrolyte was demonstrated that can perfectly comply with both fast ion adsorption on the graphite oxide cathode and co-intercalation in graphite anode. The extremely low-cost carbonaceous capacitor exhibited outstanding performance with large capacity, high rate capability, and long cyclability. Considering the cost-effectiveness, material sustainability, this new model may shed some light on searching for future energy storage devices.

MM 46.3 Wed 17:45 IFW D

Investigating the Role of Nanoarchitectured Current Collector in Supercapacitor Electrode with Thick Pseudocapacitive Materials — •Long Liu, Huaping Zhao, Mo Sha, Chenglin Zhang, Jiajia Qiu, and Yong Lei — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Pseudocapacitive materials with low electrical conductivity are mainly in the form of ultrathin conformal coating in supercapacitor electrodes based on nanoarchitectured current collectors, thus the resultant low mass loading of electroactive materials largely limits the applications of nanoarchitectured current collectors. Here, supercapacitor electrodes with nickel nanorod arrays as nanoarchitectured current collectors and MnO2 as electroactive materials are fabricated to investigate the role of nanoarchitectured current collectors in determining the energy storage capability when pseudocapacitive materials are in thick layer rather than ultrathin conformal coating. Electrochemical analysis revealed that Ni nanorods could create numerous electrical conductive tunnels in the thick-layer electrodes to dramatically alleviate the contact resistance at the electroactive-materials/current-collectors interface. Larger area capacitance, better rate capability and higher structural stability was maintained in Ni nanorods based electrodes even with thick MnO2 layer than those with Ni foils as current collectors based electrode with the same configuration. These results open up new opportunities for nanoarchitectured current collectors to construct supercapacitors with superior energy storage capability.

MM 46.4 Wed 18:00 IFW D

Phase Stability Diagrams of Group 6 Magnéli Oxides and Their Implications for Photon-Assisted Applications — •Yun-Jae Lee, Taehun Lee, and Aloysius Soon — Department of Materials Science & Engineering and Center for Artificial Synesthesia Materials Discovery, Yonsei University, Seoul 03722, Republic of Korea

Controlling the stoichiometry and metastability in functional oxides is often the key to enhancing their performance for a range of important oxide-based technological applications. In this work, using the recently developed metaGGA, SCAN+rVV10, and hybrid density-functional theory calculations, we study both stoichiometric and sub-stoichiometric (Magnéli) oxides of tungsten and molybdenum, focusing on their structural parameters, growth thermodynamics, and electronic structure for targeted photo-related applications. We report that the sub-stoichiometric Magnéli phases of tungsten oxides (namely, W_5O_{14} and $W_{18}O_{49}$) are found to be stable under both gas- and solution-based synthesis environment, while the sub-stoichiometric Magnéli phases of molybdenum oxides (namely, Mo_9O_{26}, Mo_5O_{14}, and Mo_4O_{11}) prefer to form only under gas-phase synthesis. We highlight how these n-doped sub-stoichiometric Magnéli heavy-metal oxides are indeed choice candidate materials for solar water splitting (within the Z-scheme) and as interfacial hole transport layers for the next-generation photodevices.

MM 46.5 Wed 18:15 IFW D

Lattice dynamics in PbTe under high pressure — •Zehua Li[1], Shasha Li[2], Rolf Heid[1], John-paul Castellan[3], Stefan Klotz[4], Alexandre Ivanov[5], Yue Chen[2], and Frank Weber[1] — [1]Karlsruhe Institute of Technology, Institute for Solid State Physics, 76021 Karlsruhe, Germany — [2]Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong SAR, China. — [3]Laboratoire Léon Brillouin (CEA-CNRS), CEA-Saclay, F-91911 Gif-sur-Yvette, France — [4]Sorbonne Université, UMR 7590, IMPMC, F-75252 Paris, France — [5]Institut Laue-Langevin, 71 avenue des Martyrs, 38000 Grenoble, France

Thermoelectric materials such as PbTe are interesting for energy applications as they can transform heat into useful electricity. Understanding the impact of anharmonicity in the lattice dynamical properties is the key to engineer/design new high-performance thermoelectric materials requiring a low lattice contribution to the thermal conductivity. Here, we report an investigation on zone center transverse optic phonons in PbTe at pressures up to 5.3 GPa by inelastic neutron scattering. We observe a non-monotonic pressure dependence in the phonon energy as well as a clearly reduced phonon linewidth at high pressures.