MM 54: Materials for Storage and Conversion of Energy V

Time: Thursday 10:15–11:30 Location: C 264

MM 54.1 Thu 10:15 C 264

Energy storage in a quantum battery — •Charles Downing — University of Exeter, Exeter, United Kingdom

We consider some simple theoretical models for quantum batteries, which are energy storage devices constructed using inherently quantum mechanical objects. We discuss the optimal ways to charge the battery, store energy in the battery and extract useful work from it. In particular, we show how quantum batteries display some nice non-Hermitian physics effects, in which so-called exceptional points govern the performance of the battery. We conclude by proposing some experimental platforms which could verify our theoretical predictions.

MM 54.2 Thu 10:30 C 264

chemically embedding cobalt nanospheres in N-doped carbon nanosheets for enhanced zinc-air batteries — •Ningxiang Wu[1], Huaping Zhao[1], Sheng Li[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Key Laboratory of Flexible Electronics (KLOFE) & Institute of Advanced Materials (IAM), Nanjing Tech University (NanjingTech), 30 South Puzhu Road, Nanjing, 211800, China

The next-generation oxygen electrochemical catalysts based on non-precious metals have been extensively studied for zinc-air batteries (ZABs). Among them, Co-N-C catalysts have attracted considerable attention due to their excellent oxygen catalytic performance. However, the synthesis of Co nanoparticles with uniform structure and distribution on conductive and stable substrates remains challenging. Herein, we have prepared cobalt nanoparticles chemically embedded in N-doped carbon nanosheets (Co@NCS) by a simple organic-inorganic hybrid molten salts method. Due to the multifunctional environment provided by the mixed salts, the Co@NCS can exhibit efficient oxygen reduction and evolution reaction (ORR/OER) performance, enabling them to be suitable in ZABs. The resulting ZABs have a considerable open-circuit voltage of 1.40 V, a good peak power density of 130.4 mW cm-2, and long cycle stability for 100 h at 10 mA cm-2.

MM 54.3 Thu 10:45 C 264

Electrodeposited manganese dioxide nanolayer on carbon cloth as a modified anode for improved zinc-based battery performance — •Dharani Madhavi Bundhooa, Jiajia Qiu, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Zinc-based batteries are gaining prominence as a compelling alternative to lithium-ion batteries (LIBs), driven by their safety and environmentally friendly characteristics. However, challenges associated with Zn metal anodes, particularly the formation of Zn dendrites leading to a shortened cycle life, pose obstacles to their widespread adoption. A crucial aspect in reducing dendritic deposition of Zn involves adjusting the initial uniform nucleation, which guides subsequent uniform Zn deposition. To achieve this, a nanolayer of manganese dioxide is electrodeposited onto the surface of carbon cloth, serving as active sites for controlled nucleation and growth of metal Zn. This modified anode exhibits stable cycling performance throughout repeated Zn deposition/stripping cycles. Moreover, upon assembly into full cells enhanced electrochemical performance was obtained.

MM 54.4 Thu 11:00 C 264

Tuning Structural and Electronic Properties of MOF-5 by Ligand Substitution and Metal Node Exchange — •Joshua Edzards, Holger-Dietrich Sassnick, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg, Institute of Physics, 26129 Oldenburg, Germany

Metal organic frameworks (MOFs) are novel materials with high potential in many fields of application, ranging from gas storage and catalysis to optoelectronics. MOFs are constituted by metal atoms bound together by linker molecules which can be modified by functional groups. This leads to an enormous variety of MOFs with different structural properties, which can in turn affect their electronic properties. In this project, we perform high-throughput first-principles calculations on MOF-5. We scan all possible structures that arise by exchanging Zn with metal atoms with the same oxidation state, and by substituting the linker molecule (1,4-benzodicarboxylate) with common functional groups of varying electro-donating ability. The results of 56 different structures suggest that the atomic radius of the metal node defines the lattice constant and therefore the pore size. Earth alkaline metals and hydrogen bonds caused by the ligand substitution with COOH and OH stabilize the structure the most. Ligand functionalizations mostly affect the electronic structure by tuning the gap. In particular, linker substitution with NH_2 and OH groups lead to compounds with favorable characteristics for visible-light absorption.

MM 54.5 Thu 11:15 C 264

Advancing Energy Storage: A Study on Alkali Metal-Substituted $X_3(HITP)_2$ and $X_3(HTTP)_2$ from first principles — •Sabuhi Badalov[1,2] and Harald Oberhofer[1,2] — [1]University of Bayreuth — [2]Bavarian Center for Battery Technology

This study delves into the potential of metal-organic frameworks (MOFs) as a sustainable alternate material for use in lithium-ion batteries. Specifically, we examine $X_3(HITP)_2$ and $X_3(HTTP)_2$ MOFs with alkali metal substitutions (Cu, Zn, Co, Ni) and functionalization by replacing oxygen with sulfur for $X_3(HTTP)_2$ MOFs and hydrogen with halogens (Cl, Br) and hydroxyl groups for all predicted structures.

Using density functional theory (DFT), we analyzed these MOFs' structural, electronic, and mechanical properties in both monolayer and bulk forms. Our study also utilized advanced machine learning techniques via force field (ML-FF) for vibrational calculations, accurately assessing the materials' stability and vibrational and thermal properties. By comparing our results with some reported experimental data, this research contributes to the theoretical understanding of MOFs. It offers practical applications for their use in portable electronics, electric vehicles, and renewable energy grids. Overall, this study highlights the potential of MOFs to revolutionize sustainable energy storage solutions.