MM 19: Battery Materials

Post Lithium-Ion Batteries

Time: Tuesday 10:15–11:30 Location: H 0106

MM 19.1 Tue 10:15 H 0106

Material and electrode design for sodium-ion batteries — •Yang Xu, Min Zhou, and Yong Lei — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Academic and industry interest in sodium-ion batteries (SIBs) has been resurrected in recent years, driven by the increasing market of electric vehicles and portable electronics. Sodium is one of the most abundant elements in the earth's crust and has similar chemical properties to lithium, indicating that sodium chemistry could be applied to a similar battery system to the Li counterpart. It is believed that cost-effective SIBs are an ideal replacement to lithium-ion batteries, but it requires further improvement of performance. We conduct our study of SIBs from a fundamental point of view, e.g., crystal structures, molecular structures and electrode structures, aiming at high capacity, cyclability and rate capability. Our material design has greatly promoted the performance of both inorganic (metals and oxides) and organic electrode materials, by controlling their atomic orderliness and utilizing defect chemistry. Our electrode design has proposed highly ordered nanoarrays as advanced electrode architectures to enhance surface ion availability, charge transport and electrode stability. We present here our recent work to demonstrate the material and electrode design, with the emphasis on metallic Sb and oxide-based anodes as well as organic carbonyl compounds. The design strategies could also be applicable in potassium-ion batteries.

MM 19.2 Tue 10:30 H 0106

Low-cost K0.220Fe[Fe(CN)6]0.805 as Cathode Material for Potassium-ion Batteries — •Chenglin Zhang, Yang Xu, Min Zhou, Long Liu, and Yong Lei — Institute für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, Ilmenau 98693, Germany

Benefiting from the abundance of potassium, close redox potential to lithium, and similar electrochemistry to lithium system, potassium-ion batteries (PIBs) have attracted increasing attention as an important alternative to lithium-ion batteries. Since development of PIBs is just at its infancy stage, suitable electrode materials are rather limited. We demonstrated Prussian blue K0.220Fe[Fe(CN)6]0.805 nanoparticles as a potential cathode material. It delivered a capacity of 74.5 mAh/g at 50 mA/g and a high discharge voltage of 3.1~3.4 V as well as excellent cycling stability with retention over 98% after 50 cycles. Ex-situ XRD, Raman, and XPS characterizations confirmed that the C-coordicated FeIII/FeII couple is the redox-active site and responsible for K+ storage. Furthermore, we presented a PIB full-cell by coupling the nanoparticles with commercial carbon materials. The full-cell delivered a capacity of 68.5 mAh g-1 at 100 mA g-1 and retained 93.4% of the capacity after 50 cycles. Our work highlights the potentials of future commercialization of PIBs owing to the low cost and sustainability of both electrode materials.

[1] C. Zhang, Y. Xu, M. Zhou, L. Liang, H. Dong, M. Wu, Y. Yang, Y. Lei, Adv. Funct. Mater. 2017, 1604307.

MM 19.3 Tue 10:45 H 0106

Sodium intercalation into graphite: A DFT study — •Holger Euchner[1], Anji Reddy Munnangi[1], Helen Maria Joseph[1], and Axel Gross[1,2] — [1]Helmholtz Institute for Electrochemical Energy Storage, Helmholtzstraße 11, 89081 Ulm — [2]Institute of Theoretical Chemistry, Ulm University, Albert-Einstein-Allee 11, 89069 Ulm

In contrast to graphite, disordered carbon exhibits high Na intercalation capacity and therefore may be regarded as a promising candidate for anode materials in Na ion batteries. Despite the ongoing research with respect to carbon based anodes, the underlying mechanism for Na intercalation is still strongly debated and far from being understood.

In this contribution, we present density functional theory based lattice dynamics and band structure calculations for different stages of Na intercalation in model structures of ordered and disordered graphite. Combining these calculations with data from in situ Raman scattering of Na intercalation in coconut shell derived hard carbon – and interpretation in terms of double resonant Raman scattering – allows us to provide detailed insights into the Na intercalation in disordered carbon.

MM 19.4 Tue 11:00 H 0106

Alkali metal insertion into TiO2 based ternary oxides — •Marketa Zukalova — J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, v.v.i. Dolejškova 3, CZ-18223 Prague 8, Czech Republic

The TiO2-based nanomaterials have triggered great excitement, because of their interesting structural characteristics and potential applications in energy conversion and storage. Among others, monoclinic modification of titanium dioxide (TiO2B) and Li4Ti5O12 spinel were investigated as lithium and sodium storage anode materials, Na2Ti3O7 was reported as the lowest voltage oxide material for sodium-ion batteries anode. Numerous Li insertion studies into TiO2-based materials revealed a dependency of its electrochemical behavior on morphology (particle size, surface area). In our work we demonstrate the excellent performance of sol-gel made nanocrystalline Li4Ti5O12 and Na2Ti3O7 during alkali metal insertion. Nanocrystalline Li4Ti5O12 exhibits the best performance for Na storage, its charge capacities reach 156 mAhg-1 and are twice as high as those of reference Aldrich LTS. The sol gel made Na2Ti3O7 exhibits discharge capacities of 109, 86 and 63 mAh g-1 at charging rates 1, 2 and 5C respectively, with 100% coulombic efficiency and zero capacity drop over 50 cycles after initial conditioning.

MM 19.5 Tue 11:15 H 0106

Calculation of Phase Stability and Point Defect Properties in the Perovskite $LaFeO_3$ — •Daniel Mutter[1], Daniel F. Urban[1], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]University of Freiburg, FMF, Germany

Solid oxide fuel cell (SOFC) and solid oxide electrolyzer cell (SOEC) devices, which transform chemical into electrical energy and vice versa, have the potential to make a significant contribution to the efforts of overcoming future problems of the energy economy. An optimal functionality of the electrodes in such devices requires a high catalytic activity at their surfaces, i.e. the capability for chemisorption and dissociation of O_2 molecules, charge transfer to O^{2-}, and incorporation of O^{2-} ions into vacant anion sites of the crystal structure. Promising materials regarding these requirements are perovskites (ABO_3), with La, Ba or Sr ions on the A sites, and transition-metal ions (Mn, Fe, Co) on the B sites. Using density functional theory calculations with a Hubbard-U correction, we aim to shed light on the correlation between stoichiometry, point defect concentrations and experimental synthesis conditions in the perovskite $LaFeO_3$ (LFO). The stability region of LFO in the phase diagram and point defect concentrations were calculated taking into account image charge corrections. Employing defect equilibrium reactions and applying the charge neutrality condition, point defect concentrations were obtained for varying elemental chemical potentials, i.e., synthesis conditions. The sensitivity of the results on the choice of the Hubbard-U parameter will be discussed.