MM 5: Functional Materials - Battery Materials I

Time: Monday 10:15–11:30 Location: H26

MM 5.1 Mon 10:15 H26

Charge Transfer Reactions at Electrode Materials for Lithium Ion Batteries — •Fabian Wunde, Frank Berkemeier, and Guido Schmitz — Institut für Materialphysik, Universität Münster

Powerful Lithium Ion Batteries on the one hand have to provide high energy densities, and on the other hand this energy has to be available in short period of time, i.e. they have to be capable of high charge/discharge rates. In general, these high charge/discharge rates result in both, a capacity loss and in large overpotentials. Since the hopping rate of lithium atoms, which are passing the interface between the electrode and the ion conductor, is determined by an activation energy, an external overpotential will increase the number of successful lithium transitions. In our work we studied in detail the overpotentials of ion-beam-sputtered LiFePO4 thin films, which serve as a model system. By the use of cyclic voltammetry, a linear relationship between the scan rate and the measured overpotential is observed. Solving the Butler-Vollmer equation under linear sweep boundary conditions confirms this linear behavior and finally allows us to measure the hopping rate of lithium in case of LiFePO4.

MM 5.2 Mon 10:30 H26

First-principles study of multilayer graphynes for lithium ion battery anodes — •Hoonkyung Lee — 1Division of Quantum Phases & Devices, School of Physics, Konkuk University, Seoul 143-701, South Korea

Graphynes, two-dimensional layers of sp- and sp2-bonded carbon atoms, have recently received considerable attention because of their potential as new Dirac materials. Here, focusing on their large surface area, we explore the applicability of graphynes as lithium ion battery anodes through the first-principles density functional calculations. We have found that Li potential energies are in the range suitable to be used as anodes. Furthermore, the maximum composite of Li-intercalated multilayer α- and γ-graphynes is found to be C6Li3, which corresponds to a specific capacity of 1117 mAh g-1, twice as large as the previous theoretical prediction for graphynes. The volumetric capacity of Li-intercalated multilayer α- and γ-graphynes is 1364 and 1589 mAh cm-3, respectively. Both specific and volumetric capacities of Li-intercalated graphynes are significantly larger than the corresponding value of graphite, from which we conclude that multilayer graphynes can serve as high-capacity lithium ion battery anodes.

MM 5.3 Mon 10:45 H26

Morphology and size control of LiMnPO4 nano- and microcrystals — •Christoph Neef[1], Carsten Jähne[1], Hans-Peter Meyer[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, University of Heidelberg, D-69120 Heidelberg, Germany — [2]Institut für Geowissenschaften, University of Heidelberg, D-69120 Heidelberg, Germany

A microwave-assisted hydrothermal synthesis route was applied to grow LiMnPO4 micro- and nanocrystals, starting from acetate precursors. The crystal size can be manipulated over a range of two orders of magnitude (from around 10 um down to a few 100 nm) by appropriate adjustment of both synthesis conditions: the precursor concentration and the pH-value of the reactant. The resulting crystal morphology as well as the materials texture and agglomeration tendency were investigated by means of XRD and SEM. The influence of morphology, size, and agglomeration on the electrochemical properties were investigated by cyclic voltammetry. Reversible electrochemical activity appears at particle size below 1 um.

MM 5.4 Mon 11:00 H26

Lithium Ion Transport in LCO-Li-SiO2 multilayer stacks — •Frank Berkemeier, Tobais Stockhoff, and Guido Schmitz — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm Str. 10, D-48149 Münster

Thin films of lithium cobalt oxide (LCO) and lithium silicate glass are prepared by ion beam sputter deposition. The capability of the LCO films to reversibly store and release lithium ions is proven by means of cyclic voltammetry and chronopotentiometry, while the ionic conductivity of the silicate glass is measured by electrochemical impedance spectroscopy. Furthermore, by measuring the correlation between the transmission of visible light through the LCO films and their lithium content, the intercalation/deintercalation process is studied in detail by optical transmission measurements. Applying these transmission measurements in case of LCO films of different thickness between 10 and 500 nm, allows us to determine the interface barriers for the transfer of lithium ions from the liquid electrolyte into LCO. By depositing an additional layer of silicate glass onto the LCO film, the transmission measurements are also used to obtain quantitative information about the mobility of lithium ions within the glass film.

MM 5.5 Mon 11:15 H26

Thin film batteries based on LiPON thin films — •Susann Nowak, Frank Berkemeier, and Guido Schmitz — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

We present the preparation of a complete thin film solid state lithium-ion battery by depositing a LiPON (lithium phosphorus oxynitride, $Li_3N_x(PO_4)_{1-x}$) layer between two metallic thin film electrodes on silicon. It is shown that during the first cycle of cyclic voltammetry measurements, electrochemically active interface regions are formed, serving as anode and cathode, respectively, and thus the layer stack acts as a complete electrochemical thin-film cell. These cells are investigated by means of temperature-dependent electrochemical impedance spectroscopy (EIS) and transmission electron microscopy (TEM), with special emphasis on the reactive layer between metallic electrode and LiPON. A whole typical battery (excluding the substrate) is just about 700 nm thick. To achieve such a thin geometry very smooth layer surfaces are necessary, which are prepared by reactive ion-beam sputtering of Li_3PO_4, using argon as sputter gas and nitrogen as reactive additive.

Due to their well-defined geometry, these samples are well suited to study interface reactions, with the aim to further improve lithium-ion batteries.