MM 31: Functional materials I: Supercapacitors and batteries I

Time: Wednesday 10:15–11:45   Location: H53

MM 31.1   Wed 10:15   H53

Activated Carbon-based Materials of Ultrathin Fibers — •Svetlana Klimova — Saratov State University, Astrakhanskaya 83 410012 Saratov, Russia

There is more attention to the development of new autonomous "physical" batteries with energy storage in the electric double layer (ultra-electrolytic capacitors with a dielectric layer between the electrodes (supercapacitors)). Supercapacitor is a new element of energy storage device with energy density 10 times higher than in the conventional capacitors, and pulse discharge capacity up to 10 times higher than the power batteries. High voltage (potential difference), to which the capacitor is charged and capacitance are important in energy area and improve the supercapacitor characteristics. For that present work new nonwoven materials with/without of inorganic inclusions (carbon or magnetite nanopatticles) are synthesized and modification of porous material to increase the amount of pore is obtained. The electrospinning technology provides continuous production of nanofibrous materials and was used for create a separator of supercapacitors in this work. Morphology and electric parameters were measured by the scanning electron microscope (Tescan Mira LMU II) and probe analyzer (Agilent), respectively. The application of energy storage of condenser type (ESCT) based on supercapacitor energy storage systems with nanofibrous materials makes it possible to reduce the installed capacity batteries and increase their lifetime by 1.5 - 2 times.

MM 31.2   Wed 10:30   H53

Facile synthesis of a δ-bismuth oxide/reduced graphene oxide composite and its electrochemical characteristics — •Benrong Hai, Yang Xu, Min Zhou, and Yong Lei — Institute for Physics and IMN MacroNano, Ilmenau University of Technology, Ilmenau 98693, Germany

The increasing demand for environmentally benign and economically accessible energy storage technologies has strongly promoted the need for scientific work in this area. It is currently accepted that the cubic oxide δ-Bi2O3 is one of the most promising materials which can be used as solid electrolyte in high technology equipment such as fuel cells, supercapacitors, and membrane devices which utilize the unusual high oxide ion conductivity of this metal oxide. Reduced graphene oxide is considered as the most excellent matrix to support host materials because of its promising advantages. The present work demonstrates a novel and facile route for preparing composites comprising of δ-Bi2O3 nanoparticles and graphene.

MM 31.3   Wed 10:45   H53

NMR parameter computations and the local electronic structure in oxygen-deficient LTO — •Markus Schuderer, Karsten Reuter, and Christoph Scheurer — Theoretische Chemie, Technische Universität München, Garching

Spinel-structured lithium titanium oxide $Li_4Ti_5O_{12}$ (LTO) is a promising zero-strain anode material for rechargeable lithium ion-batteries. Its relatively low electronic conductivity can be improved by introducing oxygen vacancies [1]. Experimental XPS [1] and EPR [2] results suggest the partial reduction of Ti ions. The description of the respective mixed-valent transition metal cation distribution is challenging for DFT methods. LTO's inherent stoichiometric disorder and the spatial separation of vacancies from periodic images additionally requires large supercells. We have conducted systematic studies employing PBE, DFT+U, and hybrid functionals. The expected gap states are only found in hybrid calculations. Computed quadrupolar coupling constants for Li NMR spectroscopy are correlated with lo-

cal geometric distortions and the electronic structure in the vicinity of O–vacancies, allowing for future combined theoretical and experimental NMR studies of the microscopic ion transfer pathways in this interesting material.

[1] J. Wolfenstine, U. Lee, J. L. Allen, *J. Power Sources* **2006**, *154*, 287.
[2] P. Jakes, J. Granwehr, H. Kungl, R.-A. Eichel, *Z. Phys. Chem.* **2015**, *229*, 1263.

MM 31.4   Wed 11:00   H53

^{7}Li NMR studies of lithium ion dynamics in SiOC anode materials — •Michael Haaks[1], Ralf Riedel[2], and Michael Vogel[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Germany — [2]Institut für Materialwissenschaft, Fachgebiet Disperse Feststoffe, Technische Universität Darmstadt, Germany

Rising energy demand makes it important to improve the performance of lithium ion batteries. For this purpose it is important to understand the dynamics of lithium ions, in particular, in heterogeneous materials, which are used in modern strategies for material optimization. We combine ^{7}Li NMR spin-lattice relaxation, line-shape, and stimulated-echo analyses to investigate lithium ionic motion in a polymer-derived silicon oxycarbide (SiOC) ceramic in lithiated and delithiated compounds on a broad timescale. We find that the large variety of lithium environments results in broad distributions of correlation times for the jump motion of the lithium ions. Moreover, we observe that the lithium ionic jumps are, on average, faster in the lithiated than in the delithiated compound at ambient temperatures. On the other hand, the lithiated SiOC has a higher temperature dependence of this jumps so that the difference in the ionic mobilities is reduced upon cooling. Finally, we show that heating to $400\,\mathrm{K}$ leads to irreversible changes of the prepared lithiated and delithiated samples.

MM 31.5   Wed 11:15   H53

DFT-supported study of ionic mobility in $Li_4Ti_5O_{12}$ by solid-state NMR — •Simone Köcher[1,2], Markus Schuderer[2], Magnus Graf[1], Josef Granwehr[1], Rüdiger-A. Eichel[1], Karsten Reuter[2], and Christoph Scheurer[2] — [1]IEK-9 - Fundamental Electrochemistry, Forschungszentrum Jülich, Jülich, Germany — [2]Chair for Theoretical Chemistry and Catalysis Research Center, Technische Universität München, Garching, Germany

Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful tool to gain a detailed understanding of the ionic mobility in electrolyte materials. Notwithstanding, the experimental spectra are complex and their unambiguous interpretation has to rely on independent first-principles based calculations. For studies of the ionic charge carrier mobility in $Li_4Ti_5O_{12}$ (LTO) by ^{7}Li spin-alignment echo (SAE) NMR, we provide first-principles reference values for chemical shielding and quadrupolar coupling by density-functional theory (DFT) [1] calculations. The results imply that for a quantification of ion mobility two intrinsically different influences need to be considered. On the one hand, local mobility with fast motion on the experimental timescale partially averages the NMR parameters of interest. On the other hand, global mobility by slower motion between local domains is characterized by effective, residual parameters in NMR. Therefore, the conventional interpretation of ^{6,7}Li chemical shifts and ^{7}Li quadrupolar coupling in terms of static lithium occupancy might be incomplete.

[1] C. Bonhomme *et al.*, Chem. Rev. **112**, 5733 (2012).

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