Tuesday, 24th April 2018
12.00h CIC energiGUNE
Seminar room

Host:
Dr. Juan Miguel López del Amo

Seminar: "Solid state NMR for the study of battery materials and cells"

Speaker:
Dr. Anastasia Vyalikh

From:
Institut für Experimentelle Physik, Technische Universität Bergakademie Freiberg, Freiberg, Germany

Current research efforts in the field of energy storage are directed towards improving cost and performance of lithium ion batteries as well as evaluating post lithium ion concepts. We focus on the characterisation of the structure and the ionic mobility in the NASICON-type glass-ceramic material, Li_1+xAlxGe$_2$-xP_3O_{12}, suggested as solid electrolyte for all-solid-state batteries. Using a combination of the experimental methods including ^{7}Li NMR spectroscopy and relaxometry, we enable to get insight into the physical and chemical mechanisms that govern the enhancement of Li-conductivity upon variation of its composition and glass crystallization conditions. We found that addition of yttria in certain concentration causes stabilization of polyphosphate chains and leads to sudden glass crystallization uniform in the whole volume. This specific glass structure evidently governs further crystallization behavior and ensures optimal organization of intergrain boundaries.

Despite of the extremely high theoretical gravimetric energy, practical applications of lithium-air batteries are now hindered due to limited rechargeability. Using ^{17}O isotope-enriched oxygen gas and a high magnetic field facilitates application of solid-state ^{17}O NMR for determining the discharge products such as lithium peroxide and lithium carbonate formed on a carbon electrode as a result of battery cycling.

Chemical modification of carbon materials is a well-established approach to create advanced anode materials in terms of performance, safety, cost efficiency and environmental issues. We provide a multi-scale characterization of a ^{13}C-enriched fine-grained graphitic material and its modifications through a high-temperature high pressure annealing and a room-temperature chemical treatment. We show that a high degree of ^{13}C isotope enrichment, as well as good long-term performances in Li-ion batteries, and, in particular, an improved NMR spectral resolution in the bromine-treated sample provide these materials to be suitable candidates for operando ^{13}C NMR studies of processes in electrochemical cells.

Deep understanding of electrochemical processes requires quantitative information on a molecular level, on the one hand, and with temporal resolution, on the other hand. In our studies we apply ex-situ high-resolution MAS NMR analysis in combination with in-situ NMR, in order to characterize the electrochemical intermediates, reaction products and surface microstructures in operating cells. Using in-situ NMR, formation of quasi metallic-clusters, stable electrolyte interface and surface microstructures in the operating cell with vanadium oxide as cathode was demonstrated.