MM 12: Materials for Storage and Conversion of Energy III

Time: Monday 15:45–16:45 Location: C 264

MM 12.1 Mon 15:45 C 264

The EFG Rosetta Stone: Translating between DFT simulations and Solid State NMR experiments — •Javier Valenzuela Reina[1], Simone Köcher[2,1], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Institute of Energy and Climate Research (IEK-9), Forschungszentrum Jülich

Solid-state Nuclear Magnetic Resonance (NMR) spectroscopy is an accurate, non-destructive method for the analysis of solid-state materials. However, the spectra of complex compounds, like battery materials, are usually challenging to interpret, due to disorder or amorphous phases. Predictive-quality simulations of NMR observables are therefore crucial for an unambiguous interpretation. Unfortunately, calculating NMR properties of solid-state materials is a non-trivial task. This holds particularly for the battery-relevant quadrupolar ^{7}Li isotope, which experiences additional interactions between the nuclei and the surrounding electric field gradient (EFG).

In this work, we evaluate the performance of plane-wave density-functional theory (DFT) to compute the quadrupolar coupling constants (C_Q) and asymmetry parameters (η) of different lithium salts. The impact of unit cell size, geometry, and details of the simulation strategy is assessed, and the accuracy of the results is compared to NMR of other nuclei such as aluminium.

The reference scale we thereby introduce is a valuable resource for interpreting and validating further NMR experiments and simulations.

MM 12.2 Mon 16:00 C 264

Application and pitfalls of self-measured EELS standards on a Cu based MeOH catalyst for oxidation state determination — •Daniela Ramermann, Lukas Pielsticker, Michael Poschmann, Christoph Göbel, Elisabeth H. Wolf, Holger Ruland, and Walid Hetaba — Max-Planck-Institut für Chemische Energiekonversion, Mülheim (Ruhr)

Electron energy loss spectroscopy (EELS) is a powerful technique, not only for the determination of the elemental composition, but also for the investigation of chemical bonding and oxidation states. For the analysis of EELS data, the use of cross-section models is quite common. However, the use of reference spectra (standards) improves the quantification results and in addition allows for the fitting of the edge shapes to investigate phase composition / oxidation states. Such standards are obtained from acquired materials of well-known and defined properties. There are several databases for EELS references [1], however, their content is not exhaustive.

To apply this principle on our samples, we obtained a set of well-defined materials for the acquisition of EELS reference data. As these materials may have local impurities and differ from the desired oxidation state, it is crucial to ensure that these materials are in a well-defined state. We show the process of acquiring suitable EELS standards for materials used in catalysis and the application of mapping the oxidation state and phase composition on a Cu based methanol synthesis catalyst.

[1] https://eelsdb.eu, https://eels.info/atlas, http://eel.geri.re.kr

MM 12.3 Mon 16:15 C 264

Piezoresponse force microscopy on BaTiO$_3$ based relaxors — •Markus Kratzer[1], Philipp Münzer[1], Christian Maier[3], Klaus Reichmann[3], Marco Deluca[2], and Christian Teichert[1] — [1]Chair of Physics, Montanuniversität Leoben, Leoben, AUT — [2]Materials Center Leoben, Leoben, AUT — [3]Institute for Chemistry and Technology of Materials, TU Graz, Graz, AUTGraz,

Electrical energy storage systems with high energy- and power density are of great interest in electronics. A possible material choice to realize such devices are relaxor ceramics. Lead-free examples are BaTiO$_3$ based systems, where the relaxor behavior is obtained via the disruption of the ferroelectric long-range order by replacing Ti^{4+} by homo- or heterovalent substitutes in BaTiO$_3$'s perovsike unit cell. Here, the microscopic ferroelectric behavior of BaTiO$_3$ with increasing amounts of Zr^{4+} and Nb^{5+} has been investigated utilizing piezo response force microscopy. The investigations reveal that the disruption of the ferroelectric long-range order is highly sensitive to the amount and type of substitutes.

MM 12.4 Mon 16:30 C 264

Chlorine-induced high-temperature corrosion of superheater steels — •Matthias Kroh, Georg Krupkov, Sebastian Pentz, and Ferdinand Haider — Univ. Augsburg, Inst. f. Physik, 86159 Augsburg

The combustion process in waste-incineration-plants releases a variety of chemical substances into the gas stream. Under the operational environment Cl2 and HCl cause the Chlorine-catalysed high-temperature corrosion, which is a driving factor in the degradation of the overheater tubes necessary for power generation. Literature suggests that molecular Chlorine is the far more aggressive species, although the conducted studies were of a more qualitative nature and did not take the real conditions in power plants into consideration. To further distinguish the effect of the two species either HCl or Cl2 was let flow directly into the setup. Thereby the Cl2 was produced using a Chlorine generator, in which the reaction of liquid NaOCl and H2SO4 releases Cl2 in the process. The Chlorine concentrations were quantified by GCMS and UV VIS spectrometry, whilst the concentration of HCl was quantified through ISE measurements. In these experiments the corrosive attack of Cl2 and that of HCl on samples of a typical superheater steel was determined for various temperatures and defined gas atmospheres. The experimental setup consists of a horizontal furnace, where the samples were exposed to a flow of the desired gas atmosphere, followed up by a gas analysis. Weight loss of the samples after removing reaction products as well as the morphology of the reaction zone are determined after various exposure times.