MM 28: Transport & Diffusion III

Time: Tuesday 15:00–16:00 Location: H26

MM 28.1 Tue 15:00 H26

^{7}Li NMR field-cycling relaxometry: A powerful tool to investigate lithium ion dynamics in solid-state electrolytes — •Jan Gabriel, Magnus Graf und Michael Vogel — Institut für Festkörperphysik, Technische Universität Darmstadt, Germany

We use ^{7}Li NMR to study lithium ion dynamics in glasses like (Li_2S)-(P_2S_5) and (Li_2S)-(GeS_2)-(GeO_2). Field-cycling relaxometry is employed in combination with stimulated-echo experiments and line shape analysis to cover a time window extending over 10 orders of magnitude. The stimulated-echo method is suitable to measure the correlation functions $F_2(t)$ of lithium ion dynamics in solids in a time range from 10^{-5} to 10^1 s. Field-cycling relaxometry measures the spectral density $J_2(\omega)$ from which we obtain a correlation function in a range from 10^{-9} to 10^{-5} s. The motional narrowing of NMR spectra is sensitive from 10^{-4} to 10^{-5} s. These three methods probe translational motion of the lithium ions. The field-cycling and stimulated-echo data revealed a nonexponentiality of the lithium ion dynamics in the studied glasses. The shape of the spectral density $J_2(\omega)$ is well described by a Cole-Davidson function and the decay of the correlation function of $F_2(t)$ is well interpolated by a Kohlrausch-William-Watts function. Observation of the T_1 minimum for a broad range of Larmor frequencies allows us to determine temperature-dependent correlation times and, thus, the activation energy of lithium ion dynamics. When the dynamics of the lithium ions is too slow to be observed at sufficiently low temperatures, field-cycling relaxometry probes the nearly constant loss, which is considered as a universal phenomenon of disordered solids.

MM 28.2 Tue 15:15 H26

Majorana fermions from Landau quantization in a superconductor-topological insulator hybrid structure — •Rakesh P Tiwari[1], Ulrich Zuelicke[2], and Christoph Bruder[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]School of Chemical and Physical Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, PO Box 600, Wellington 6140, New Zealand

We show that the interplay of cyclotron motion and Andreev reflection experienced by massless-Dirac-like charge carriers in topological-insulator surface states generates a Majorana-particle excitation. Based on an envelope-function description of the Dirac-Andreev edge states, we discuss the kinematic properties of the Majorana mode and find them to be possible to be tuned by changing the superconductor's chemical potential and/or the magnitude of the perpendicular magnetic field. Our proposal opens up new possibilities for studying Majorana fermions in a controllable setup.

MM 28.3 Tue 15:30 H26

Thermoelectric Transport Coefficients from First Principles — •Karsten Rasim, Christian Carbogno, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, Berlin, Germany

Significant effort is currently being invested in the search and optimization of thermoelectric (TE) materials, which promise ecologic and economic impact for waste-heat recovery [1]. Respective first-principles studies of the TE transport coefficients have almost exclusively relied on the Boltzmann-transport framework; the electron-phonon coupling is thereby accounted for within first-order perturbation theory [2]. However, such approaches become increasingly questionable at high temperatures due to anharmonic effects and do not allow the assessment of the Seebeck coefficient. The Greenwood-Kubo (GK) method, which includes those effects via *ab initio molecular dynamics*, does not suffer these limitations and provides access to all electronic transport coefficients even at high temperatures. In fact, it has hitherto been used for matter under extreme thermodynamic conditions, e.g, for melts and plasmas [3], but not for condensed materials. We demonstrate and analyze the applicability of the GK method for TE compounds, discuss the required adaptations, the accuracy and the limits of this approach by computing the transport coefficients for direct/indirect band gap semiconductors.

[1] G. J. Snyder and E. S. Toberer, Nature Mat. **7**, 105-114 (2008)
[2] P. Boulet and M. J. Verstraete, Comp. Mat.Sci. **50**, 3 (2001)
[3] V. Recoules and J.-P. Crocombette, Phys. Rev. B **72**, 104202 (2005).

MM 28.4 Tue 15:45 H26

Ab initio study of ionic mobility in anisotropic zirconia — •Julian Hirschfeld and Hans Lustfeld — Forschungszentrum Jülich, IAS-1 and PGI-1, Jülich, Germany

Electrolytes with high ionic mobility at lower temperatures are the prerequisite for the success of Solid Oxide Fuel Cells (SOFC). One candidate is Yttrium Stabilized zirconia (YSZ). In the past the ionic resistance of YSZ electrolytes has mainly been decreased by reducing their thickness. But this decreases the resistance only linearly. However, the migration barriers of the oxygen ions influence their mobility exponentially. Recently it has been shown that those barriers can be reduced by applying negative [1] or strong positive [2] pressure.

Here we proceed as follows: Since the ionic motion needs to be good in transport direction only, we have freedom in investigating anisotropic structures. And we have found a peculiar one which - according to density functional (DFT) computations, combined with the Nudged Elastic Band (NEB) method and molecular dynamics (MD) computations - has the potential to outperform YSZ.

[1] T. J. Pennycook et al., PRL 104, 115901 (2010) [2] J. A. Hirschfeld and H. Lustfeld, PRB 84, 224308 (2011)