MM 26: Transport in Materials: Diffusion, Charge, or Heat Conduction I

Time: Wednesday 15:45–17:00 Location: SCH/A216

MM 26.1 Wed 15:45 SCH/A216

Theoretical investigation of the conductivity of the $LiMnPO_4$ Battery Material — •Franz Winkler and Harald Oberhofer — Chair for Theoretical Physics VII and Bavarian Center for Battery Technologies, University of Bayreuth

Developing better batteries and thus battery materials is a crucial step in humanity's urgent energy transition. Thereby, theory can play an important role in characterizing and understanding the properties of the involved materials. In this contribution we present our work on olivine $LiMnPO_4$ which exhibits some desirable properties such as a high energy density and a high potential and thus operating voltage. However, its adoption is hampered by a bad conductivity. In order to understand the barriers to conductivity and suggest potential remedies we compute electronic and ionic transport properties and how they could be influenced by defects.

The electron and hole band transport mobilities are calculated using Hubbard-corrected electronic density functional theory (DFT+U), both for antiferromagnetic and paramagnetic $LiMnPO_4$ as well as materials derived by substitution. For ionic conductivity we determine the minimal energy path of the Li ions via the nudged elastic band (NEB) method. To reduce calculational cost and enable larger systems, we use machine learned force fields and refine these models via DFT to transition states. Li ions are transported in $LiMnPO_4$'s 1D channels. However these diffusion paths can be blocked by antisite defects. As those very strongly limit ionic transport we investigate their stability with first-principle DFT, phonon and thermodynamics calculations.

MM 26.2 Wed 16:00 SCH/A216

Multiscale modeling of cooperative defect dynamics in MoS_2 — •Aaron Flötotto[1,2], Erich Runge[1,2], and Christian Dressler[1,2] — [1]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — [2]Technische Universität Ilmenau, Institut für Mikro- und Nanotechnologien, Ilmenau, Germany

Chalcogen vacancies strongly influence the electrical and memristive properties of transition metal dichalcogenides including MoS_2. However, capturing their dynamics at device-relevant time and length scales is challenging due to the high energy barriers associated with individual atomic jumps [1]. We have developed a multiscale framework for MoS_2 that uses *ab-initio* molecular dynamics to generate training data for machine-learning force fields. This step reveals the motifs of cooperative sulfur-vacancy migration and cluster formation [2]: (i) Vacancy migration almost exclusively occurs by vacancy-assisted hopping, implying non-linearities and suggesting memristive behavior; (ii) An energy barrier comparable to lab temperatures protects long vacancy lines against splitting into smaller vacancy clusters.

These insights are incorporated into a Monte-Carlo model that reproduces several key experimental observations and enables the prediction of device level quantities, such as the vacancy-density-dependence of the diffusion coefficient of sulfur vacancies in MoS_2.

[1] Q. Chen, et al. , ACS Nano 12, 7721-7730 (2018), doi: 10.1021/acsnano.8b01610.

[2] A. Flötotto, et al., arXiv:2508.13790 (2025).

MM 26.3 Wed 16:15 SCH/A216

Coupled Spin–Orbital–Lattice Interactions in FeO: A DFT+U and Heisenberg Analysis — •Hao Chen, Christoph Freysoldt, Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Nachhaltige Materialien GmbH, Düsseldorf, Germany

Wüstite (FeO) is a prototypical correlated oxide where spin, orbital, and lattice degrees of freedom are intricately coupled. In addition, significant deviations from stoichiometry can occur via oxygen vacancies and Fe^{2+}/Fe^{3+} mixed valency. Local lattice distortions and orbital reorientations around such defects can modify magnetic exchange pathways and thus the defect formation energies. Using DFT+U, we investigate how the orbital orientation in Fe^{2+} correlates with structural strain and magnetic interactions. Our results reveal a well-defined correlation between the minority-spin t_{2g} occupation and the rhombohedral distortion parameter, giving rise to four distinct symmetry-broken orbital states. By mapping total-energy differences between these orbital configurations onto an effective Heisenberg model, we show that the exchange constants are sensitive to orbital orientation, evidencing strong superexchange–orbital coupling. This framework provides quantitative insight into the competition between Jahn–Teller-like lattice distortions and anisotropic magnetic exchange arising from orbital orientation. Building on this, the study provides a unified DFT+U-based picture of spin–orbital–lattice coupling in FeO and establishes a consistent energetic framework for incorporating spin and orbital effects into defect calculations.

MM 26.4 Wed 16:30 SCH/A216

Quantum interference in higher pseudospin fermions — •Gargee Sharma and Arpan Gupta — Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016 India

We construct a unified theory of quantum-interference corrections in disordered pseudospin-s fermions described by $k\cdot\mathbf{S}$ Hamiltonians. Employing the rotation-group structure of SU(2), we derive closed-form wavefunctions, scattering and vertex corrections, and Cooperon kernels valid for arbitrary pseudospin s in two and three dimensions. A universal "parity rule" emerges: integer s (orthogonal symmetry, $T^2 = +1$) yields weak localization, half-integer s (symplectic, $T^2 = -1$) yields weak antilocalization, while interband and intervalley scattering renormalize the prefactor via a finite Cooperon-mass matrix. Explicit results for $s = \frac{1}{2}$ and $s = 1$ reproduce graphene and spin-1 Weyl limits and verify the general scaling laws. Our approach resolves the long-standing ambiguity in interband scattering, providing an analytic route for arbitrary s and concrete predictions for multifold-fermion materials.

MM 26.5 Wed 16:45 SCH/A216

Effects of strong electron-electron interactions on the conductivity of free-standing graphene — •Maksim Ulybyshev[1], Adrien Reingruber[1], and Kitinan Pongsangangan[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Würzburg, Germany — [2]Department of Physics, Faculty of Science, Mahidol University, Bangkok, Thailand

Transport in strongly correlated systems is often described using the Boltzmann equation, where correlation effects enter through the collision integral. In practice, the collision integral is usually evaluated with a number of approximations, such as computing scattering amplitudes only up to tree-level diagrams. These approximations become unreliable when interactions are sufficiently strong.

Free-standing graphene provides a representative example, as the effective coupling constant of its low-energy effective field theory exceeds unity. Using unbiased Quantum Monte Carlo (QMC) simulations on lattices with up to 102x102 unit cells and long-range Coulomb interactions, we investigate both the DC and optical conductivity of free-standing graphene. We find that the optical conductivity remains essentially unaffected by interactions, whereas the DC conductivity exhibits a strong dependence on both temperature and interaction strength. We then compare these results with kinetic-theory calculations based on the Boltzmann equation, highlighting how the QMC data can guide improvements in the accuracy of the collision integral.