MM 28: Transport in Materials: Diffusion / Electrical Transport & Magnetism

Time: Thursday 10:15–11:30 Location: H44

MM 28.1 Thu 10:15 H44

Electrical resistivity of magnetron-sputtered $Fe_{1-x}O$ thin films — •Simon Evertz[1], Nina Nicolin[1], Daniel Primetzhofer[2], James P. Best[1], and Gerhard Dehm[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — [2]Department of Physics and Astronomy, Uppsala University, S-75120 Uppsala, Sweden

$Fe_{1-x}O$ (wüstite) is a critical phase for a number of applications in the future hydrogen economy, such as photochemical materials for H_2 production by water-splitting. Hence, charge transport is crucial for the applicability of $Fe_{1-x}O$ in electrode materials. To probe the charge transport of close-to-stoichiometric $Fe_{1-x}O$, thin films were synthesized by reactive magnetron sputtering with systematically varied O_2 gas flow. The phase formation and chemical composition was correlated to the electrical resistivity and mechanical properties, as measured in a van-der-Pauw-setup and nanoindentation, respectively. The charge transport mechanism is shown to change from thermally activated hopping of charge carriers - typical for a semiconductor - to metallic-like behavior as a function of the phase purity of the films. By correlative analysis of phase purity, microstructure and mechanical properties, it is shown that already small amounts of Fe as impurity phase are decisive for changing the charge transport mechanism. These significant changes in charge transport are further compared to the hardness and Young's modulus of these films.

MM 28.2 Thu 10:30 H44

Electronic structure and transport properties of NdTe3 — Kirstine J Dalgaard[1], Shiming Lei[1], Claudius Müller[2], Steffen Wiedmann[2], Martin Bremholm[3], and •Leslie M Schoop[1] — [1]Department of Chemistry, Princeton University, Princeton, NJ, USA — [2]High Field Magnet Laboratory (HFML-EMFL), Radboud University, Nijmegen, Netherlands — [3]Department of Chemistry, Aarhus University, Aarhus, Denmark

The delocalized, hypervalent bonding in some main group element square-net materials have been linked to fascinating phenomena, including band inversions with high charge carrier mobility, and topologically nontrivial band structures. The family of rare earth tritellurides crystalize in a van der Waals structure with double tellurium square-nets, where the tellurium p orbitals form the Fermi energy crossing bands, and the partly filled 4f orbitals give rise to a rich spectrum of magnetic properties. The tellurium square-nets also undergo incommensurate charge density wave transitions affecting the band structure in ways that are yet to be fully understood. In this work, we studied the electronic structure of neodymium tritelluride through quantum oscillation and transport measurements. A remarkably high electron mobility for a magnetic van der Waals material was found, suggesting steeply dispersed bands, along with thus far unreported deviations from conventional Lifshitz-Kosevich behavior.

MM 28.3 Thu 10:45 H44

Non-coplanar magnetism, topological density wave order and emergent symmetry at half-integer filling of moiré Chern bands — •Patrick Wilhelm[1], Thomas Lang[1], Mathias Scheurer[1], and Andreas Läuchli[1,2,3] — [1]Institut für Theoretische Physik, Universität Innsbruck, 6020 Innsbruck, Austria — [2]Laboratory for Theoretical and Computational Physics, Paul Scherrer Institute, 5232 Villigen, Switzerland — [3]Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

We study the impact of Coulomb interactions at half-integer filling of the moiré Chern bands of twisted double-bilayer graphene and twisted mono-bilayer graphene, using unbiased exact diagonalization complemented by unrestricted Hartree-Fock calculations. For small intra-sublattice tunneling, wAA, a non-coplanar magnetic state is found which has the same symmetries as the tetrahedral antiferromagnet of the triangular moiré lattice and can be thought of as a skyrmion lattice commensurate with the moiré scale. The antiferromagnetic order competes with a set of ferromagnetic, topological charge density waves, which are favored for larger wAA and are associated with an approximate emergent O(3) symmetry, 'rotating' the different charge density wave states into each other. Exhibiting a finite charge gap and Chern number C=|1|, the formation of charge density wave order which is intimately connected to a skyrmion lattice phase is consistent with recent experiments on these systems.

MM 28.4 Thu 11:00 H44

Interference effects in one-dimensional moiré crystals — •Nils Wittemeier[1], Matthieu J. Verstraete[2,4], Pablo Ordejón[1], and Zeila Zanolli[3,4] — [1]Catalan Institute of Nanoscience and Nanotechnology, ICN2 (CSIC, BIST), Bellaterra, Spain — [2]NanoMat/Q-Mat/CESAM, Université de Liège (B5), Liège, Belgium — [3]Chemistry Department & Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, the Netherlands — [4]ETSF

This work [1] investigates interference effects in finite sections of 1D moiré crystals using the Landauer-Büttiker formalism within the tight-binding approximation. We explain interlayer transport in double-wall carbon nanotubes and demonstrate that wave function interference is visible at the mesoscale: in the strong coupling regime, as a periodic modulation of quantum conductance and emergent localized states; in the localized-insulating regime, as a suppression of interlayer transport, and oscillations of the density of states. The interlayer transmission between strongly coupled metallic nanotubes is limited to either $1G_0$ or $2G_0$. Our results could be exploited to design quantum electronic devices, e.g. nonelectric switches based on chiral nanotubes. Most importantly, we clarify the origin of the so-far unexplained $1G_0$ quantum conductance measured in multi-wall carbon nanotubes [2, 3].

[1] N. Wittemeier *et al.* Carbon **186**, 416 (2022)
[2] S. Frank *et al.* Science **280** (1998)
[3] W. A. de Heer & C. Berger, Phys. Rev. Lett. **93**, 259701 (2004)

MM 28.5 Thu 11:15 H44

On correlations between local chemistry, distortions and kinetics in high entropy nitrides: an ab initio study — •David Holec[1], Ganesh K. Nayak[1], Andreas Kretschmer[2], Paul H. Mayrhofer[2], Marcus Hans[3], and Jochen M. Schneider[3] — [1]Department of Materials Science, Montanuniversität Leoben, Leoben, Austria — [2]Institute of Materials Science and Technology, TU Wien, Vienna, Austria — [3]Materials Chemistry, RWTH Aachen University, Aachen, Germany

High entropy alloys (HEAs) have triggered significant scientific interest due to their unusual structural stability combined with excellent mechanical and other functional properties. Recently, exploration of materials used as protective coatings has also entered this room by exploring high entropy borides, oxides, carbides, and nitrides. These chemically complex systems provide huge combinatorial space for tuning the composition, hence making the experimental exploration tedious. High-throughput simulations based on unbiased ab initio calculations provide an ideal tool to guide the experiments.

We will show that for high entropy nitrides (HENs), strain is equally important for the stabilization as entropy. Our predictions were validated by experimental investigations on the thermal stability of selected HEN coatings. The predicted structures are further characterized in terms of their local distortions, one of the core effects of HEAs. Another core effect is sluggish bulk diffusion. Therefore, in the second part of the talk, we will explore correlations between migration barriers for bulk diffusion, local chemical compositions, and local distortions.