

MM 22: Functional Materials IV: Thermoelectric and Multiferroic Materials

Time: Tuesday 10:15–11:45

Location: TC 010

MM 22.1 Tue 10:15 TC 010

Thermoelectric properties of the layered rhodates K_xRhO_2 and Na_xRhO_2 — •UDO SCHWINGENSCHLÖGL, YASIR SAEED, and NIRPENDRA SINGH — KAUST, Thuwal 23955-6900, Saudi Arabia

The thermoelectric properties of the layered oxides K_xRhO_2 ($x = 1/2$ and $7/8$) are investigated by means of the electronic structure, as determined by *ab initio* calculations and Boltzmann transport theory. In general, the electronic structure of K_xRhO_2 is similar to Na_xCoO_2 , but with strongly enhanced transport. $K_{7/8}RhO_2$ exceeds the ultra-high power factor of $Na_{0.88}CoO_2$ reported previously by more than 50%. The roles of the cation concentration and the lattice parameters in the transport properties in this class of compounds are explained. In addition, we study the 3R phases of Na_xRhO_2 for different Na vacancy configurations and concentrations. As compared to the analogous 2H phases, the modified stacking of the atomic layers in the 3R phases reduces the interlayer coupling. As a consequence, the 3R phases are found to be superior in the technologically relevant temperature range. The Rh $d_{3z^2-r^2}$ orbitals still govern the valence band maxima and therefore determine the transport properties. A high figure of merit of 0.35 is achieved in hydrated $Na_{0.83}RhO_2$ at 580 K by water intercalation, which is 34% higher than in the non-hydrated phase. References: Adv. Funct. Mater. 22, 2792 (2012); Sci. Rep. 4, 4390 (2014).

MM 22.2 Tue 10:30 TC 010

Thermoelectric properties of individual Ag nanowires under the terms of quasiballistic transport — •RÜDIGER MITDANK¹, DANNY KOJDA¹, ZHI WANG², JOHANNES RUHHAMMER², PETER WOLAS², and SASKIA F. FISCHER¹ — ¹AG Neue Materialien, Humboldt Universität zu Berlin, D-12489 Berlin, Newtonstr. 15 — ²Laboratory of Design of Microsystems, University of Freiburg, IMTEK, D-79110 Freiburg

The thermoelectric properties of Ag nanowires (NW) are discussed as a function of temperature T. Especially the electrical conductivity and the thermal conductivity showed reduced values with respect to the bulk. The latter are both notably dominated by surface scattering due to an increased surface-to-volume ratio. By lowering T, the electron mean free path strongly exceeds the NW's diameter of 150nm so that the transition from diffusive transport to quasi ballistic transport is observed. Whereas the conductivities are influenced by the NW's diameter the Lorenz number $L(T)$ turns out to be independent of surface scattering. Instead of that, the characteristic of $L(T)$ is determined by the material's purity. Moreover, the temperature dependence of the electrical conductivity and $L(T)$ can be described by the bulk Debye temperature of silver.

MM 22.3 Tue 10:45 TC 010

Vibrational dynamics of filled skutterudites: Role of the fillers — •SUSMITA BASAK, CHRISTIAN CARBOGNO, and MATTHIAS SCHEFFLER — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Skutterudites are regarded as potential candidates for next-generation thermoelectric materials for electrical power generation using either solar energy or waste heat [1,2]. They form open cage-like covalent structures with large interstitial voids that can accommodate filler atoms. In principle, the thermoelectric efficiency of skutterudites can be tailored and improved in presence of these foreign atoms because different filler species affect the vibrational and electronic transport coefficients differently. In order to rationalize this phenomenon, various (in part mutually exclusive) mechanisms (rattling of filler atoms [3], hybridization between guest and host atoms [4] etc.) have been evoked in literature. To shed light on the underlying interactions, we use density functional theory to systematically study the electronic

structure and the lattice dynamics of skutterudites ($CoSb_3$, $CoAs_3$ etc.) with various fillers (Ba, Ga, In, Sn etc.). We incorporate the full anharmonicity of the inter-atomic interactions via *ab initio* molecular dynamics techniques. Our calculations reveal a unified mechanism that determines the dynamics and hence provide insights/guidelines to engineer the vibrational band structure in this material class.

[1] B. C. Sales *et al.*, Science **272**, 1325 (1996). [2] G. S. Nolas *et al.*, Phys. Rev. B, **58**, 164 (1998). [3] G. A. Slack *et al.*, J. Appl. Phys. **76**, 1665 (1994). [4] J. L. Feldman *et al.*, Phys. Rev. B **61**, R9209 (2000).

MM 22.4 Tue 11:00 TC 010

Microscopic model of paraelectric/ferroelectric perovskites — •GIOVANNI PIZZI¹, ANDREA CEPPELOTTI¹, BORIS KOZINSKY², and NICOLA MARZARI¹ — ¹Theory and Simulation of Materials (THEOS) and National Center for Computational Design and Discovery of Novel Materials (MARVEL), EPFL (CH) — ²Robert Bosch LCC Research and Technology Center, Cambridge (USA)

Even if ferroelectric materials like $BaTiO_3$ have been used for decades in a broad range of technological applications, there is still significant debate in the literature concerning their microscopic behavior. In particular, many perovskite systems display a high-temperature cubic phase with zero net polarization, whose microscopic nature is though still unclear. Indeed, some of these perovskite systems display a complex energy landscape with multiple local minima. Using our high-throughput platform AiiDA (www.aiida.net) to manage all calculations, we perform a study on a set of representative ABO_3 perovskites. We use spacegroup techniques to systematically analyze all possible local displacement patterns that are compatible with a net paraelectric phase, together with DFT calculations to assess the energetics and the stability of these patterns. Using this technique, we are able to describe the different classes of microscopic models underlying the perovskite systems.

MM 22.5 Tue 11:15 TC 010

Design of a Mott Multiferroic from a Non-Magnetic Polar Metal — •GIANLUCA GIOVANNETTI¹, DANILO PUGGIONI², JAMES RONDINELLI², and MASSIMO CAPONE¹ — ¹CNR-IOM-Democritos National Simulation Centre and International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136, Trieste, Italy — ²Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104, USA

Metals are expected to not exhibit ferroelectricity because static internal electric fields are screened by conduction electrons. A class of materials known as "ferroelectric metals" was discussed theoretically by Anderson and Blount in 1965 [1]. Recently $LiOsO_3$ has been found to be a "ferroelectric metal" in the sense that it is a metal but it develops a broken-symmetry ionic structure [2]. Using a combined approach based on Density Functional Theory and Dynamical Mean Field Theory we address the driving force behind the ferroelectric instability in metallic $LiOsO_3$ and we show that the metallic state of $LiOsO_3$ is controlled by the amount of the electronic correlations of the t_{2g} states of Os. We unveil how the effect of correlations of this compound can be tuned to engineer a Mott Multiferroic state in Li_2NbOsO_6 1/1 superlattice. We find Li_2NbOsO_6 1/1 superlattice to be a type-II multiferroic material with large ferroelectric polarization and Néel temperature close to room temperature.

[1] Anderson and Blount, Phys. Rev. Lett. **14**, 217 (1965). [2] Y. Shi *et al.* Nat. Mat. **12**, 1024 (2013).

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