# HL 48: Thermoelectricity

Time: Thursday 17:00–18:00 Location: EW 015

HL 48.1 Thu 17:00 EW 015

**Ab-initio calculations of the thermoelectric properties of MXenes** — •Udo Schwingenschlögl, Appala Naidu Gandi, and Sonu Kumar — King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

Ab-initio calculations are used to study the MXenes $Ti_2CO_2$, $Zr_2CO_2$, and $Hf_2CO_2$ in order to evaluate the role of the metal atom for the thermoelectric properties. The lattice thermal conductivity is demonstrated to grow along the series Ti-Zr-Hf in the temperature range 300-700 K, resulting in the highest figure of merit in the case of $Ti_2CO_2$. Flat conduction bands promote the thermopower in the case of n-doping. Functionalization effects are studied for $Sc_2C$, which is semiconducting for various functional groups, including O, F, and OH. The lowest lattice thermal conductivity is found for OH functionalization. Despite a relatively low thermopower, $Sc_2C(OH)_2$ therefore and due to a high electrical conductivity can be interesting for intermediate-temperature thermoelectric applications. We also discuss results on heterostructures built of MXenes and transition metal dichalcogenide monolayers. Low frequency optical phonons are found to occur as a consequence of the van der Waals bonding. They contribute significantly to the thermal transport and compensate for reduced contributions of the acoustic phonons (strong scattering in heterostructures), such that the thermal conductivities become similar to those of the constituent MXenes. References: Chem. Mater. **28**, 1647 (2016); Phys. Rev. B **94**, 035405 (2016); J. Phys.: Condens. Matter **29**, 035504 (2017).

HL 48.2 Thu 17:15 EW 015

**Half-Heusler materials : predictions from density functional theory and many-body perturbation theory** — •Maedeh Zahedifar and Peter Kratzer — University Duisburg-Essen

For harvesting waste heat at elevated temperature ( T > 400 K), ternary materials with crystal structure $C1_b$, so-called half-Heusler alloys, have attracted much attention due their high thermal stability and their environmental friendliness. Different exchange correlation functionals (GGA-PBE, HSE06) and the GW approach are used to investigate the effects of these approaches on the band structures and effective masses of six half-Heusler materials with chemical formula ANiSn and ACoSb (A = Zr, Hf and Ti). The GW approach is recommended for Sb compounds in particular, because not only does the position of the valence band maximum change from $\Gamma \rightarrow L$, but also it strongly affects in thermoelectric properties. In Sn compounds, the conduction band effective mass is underestimated by the HSE06 functional (compared with the GW calculation), but for Sb materials, HSE06 calculations are closer to GW results. Of the six investigated materials, ZrCoSb is determined to be the best thermoelectric material due to its high $ZT$. After comparing results from different methods for the considered materials, it can be concluded that the simplest method, PBE, is not enough to give conclusive results about thermoelectric properties of investigated materials.

HL 48.3 Thu 17:30 EW 015

**performance simulation of micro thermoelectric coolers** — •david alberto lara ramos — Leibniz-Institut für Festkörper- und Werkstoffforschung. Dresden. Germany

Micro thermoelectric coolers are increasingly considered as an attractive technology to meet the heat management requirements in electronic and solid state devices due to their simplicity, compact size, robustness, noise free operation, high long term reliability (due to their lack of mechanical moving parts or working fluids) and subsequently maintenance free capability and fast control response. However, due to nature of thermoelectricity, a comprehensive device performance simulation process is needed in order to fully make use of the available material properties; and this device optimization turns to be challenging due to the thermoelectricity Multiphysics environment which involves coupled electrical and heat fluxes. Furthermore, despite optimization strategies for macro thermoelectric coolers are well known, new challenges take place when designing thermoelectric coolers at the micro scale. In the present work, finite element analysis were performed in order to study the parasitic effect of the geometrical definition of a single leg pair micro thermoelectric module manufactured by available state of the art lithography and electrochemical deposition techniques. The obtained results show how the observed maximum temperature suppression and heat dissipation power, are affected by parasitic effects, such as Joule heating and heat flux across the thermoelectric leg pair.

HL 48.4 Thu 17:45 EW 015

**Understanding chemical ordering in intermetallic clathrates from atomic scale simulations** — •Mattias Ångqvist and Paul Erhart — Chalmers, Sweden

Intermetallic clathrates exhibit great variability with respect to elemental composition and distribution. While this provides a lot of flexibility for tuning properties it also poses a challenge with regard to developing a comprehensive understanding of these systems. In this study we employ a combination of alloy cluster expansions and density functional theory calculations to exhaustively sample the compositional space with *ab-initio* accuracy. Using this methodology we study chemical ordering and associated properties in the clathrate systems $Ba_8Al_xSi_{46-x}$, $Ba_8Al_xGe_{46-x}$, $Ba_8Ga_xGe_{46-x}$, and $Ba_8Ga_xSi_{46-x}$ as a function of composition and temperature. We achieve very good agreement with the available experimental data for the site occupancy factors (SOFs) even for stoichiometries beyond the composition range considered during construction of the cluster expansions. This validation enables us to resolve trends in the experimental data and explain non-monotonic variations of the SOFs. In particular, we provide a rationale for the pronounced composition dependence of the SOFs in Al based clathrates. Furthermore, we quantify the effect of chemical ordering on both heat capacity and lattice expansion. Finally, we determine the effect of chemical disorder on the displacements of the guest species (Ba), which enables us to at least partially explain experimental observations of the nuclear density of Ba in different clathrates.