MM 17: Poster Ib

Time: Monday 18:30–20:30 Location: Poster F

MM 17.1 Mon 18:30 Poster F

Implementation of Experimental Results in an Ontology of Magnetocaloric Materials Research — Simon Bekemeier[1], Moritz Blum[2], Luana Caron[3,4], Philipp Cimiano[2], Basil Ell[2], Inga Ennen[3], Michael Feige[1], Maik Gaerner[3], Thomas Hilbig[1], Andreas Hütten[3], Günter Reiss[3], Tapas Samanta[3], Sonja Schöning[1], Christian Schröder[1,3], Lennart Schwan[1,3], and •Martin Wortmann[3] — [1]University of Applied Sciences and Arts, Bielefeld, Germany — [2]Faculty of Technology and CITEC, Bielefeld University, Bielefeld, Germany — [3]Faculty of Physics, Bielefeld University, Bielefeld, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Magnetic refrigeration based on the magnetocaloric effect is an environmentally friendly alternative to compression based cooling. The cooling effect is based on heat release or uptake during magnetic phase-transitions of a magnetocaloric material. The decades-long search for alloys suitable for mass application could be made much more efficient by digitizing the scientific process chain. The project DiProMag seeks to digitalize the process chain from theory, simulation and experiment to prototypical applications in an ontology. Here, we show how experimental results are implemented in a hierarchical ontology. Various Heusler alloys have been investigated as thin films, nanostructures, and bulk material. Different approaches have been developed for these materials to be integrated into functional prototypes. The goal is to standardize data evaluation and reporting to make it more accessible and comparable across different fields within the community.

MM 17.2 Mon 18:30 Poster F

Electronic structure fingerprints of nickel-cobalt-manganese oxide from high-throughput ab initio calculations — •Timo Reents[1], Daniel Duarte-Ruiz[1], and Caterina Cocchi[1,2] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg — [2]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin

Nickel-cobalt-manganese (NCM) oxides are established cathode materials for energy storage. Their structural complexity outlines the challenges of modelling these systems in realistic stoichiometries and compositions. Ab initio methods embedded in automatized workflows are particularly suited to address this task as they provide a tool to efficiently perform quantum-mechanical calculations on multiple structures. In this work, we model possible candidates by exchanging the transition metals atoms of $LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2$ to adjust their concentration. This offers a handle to tune the structural and electronic properties of the materials to match the desired composition. By exploiting data-driven methods on top of the computed projected density of states (PDOS), we group the results into clusters and propose a scheme to relate structural properties to PDOS fingerprints. The insight gained into the distribution of different oxidation states and the local structural arrangements is utilized to interpret x-ray absorption data from synchrotron measurements. The good agreement obtained in this procedure confirms the validity of the adopted computational approach and offers excellent perspectives for their application to other classes of technologically relevant compounds.

MM 17.3 Mon 18:30 Poster F

From ab-inito to experiments: A Python workflow for constructing neuroevolution potentials — •Eric Lindgren[1], Adam Jackson[2], Zheyong Fan[3], Christian Müller[4], Jan Swenson[1], Thomas Holm-Rod[5], and Paul Erhart[1] — [1]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Centre for Sustainable Chemical Technologies and Department of Chemistry, University of Bath, United Kingdom — [3]College of Physical Science and Technology, Bohai University, Jinzhou, People's Republic of China — [4]Department of Chemistry and Chemical Engineering, Chalmers University of Technology, Gothenburg, Sweden — [5]ESS Data Management and Software Center, Copenhagen, Denmark

Neuroevolution potentials, NEPs, as implemented in the GPUMD package are a highly accurate and computationally efficient type of machine-learned interaction potentials, enabling large scale MD simulations with system sizes up to millions of atoms with ab-initio level accuracy. Here, we present a Python workflow for constructing and sampling NEPs using the 'calorine' package, and how the resulting trajectories can be analysed with the 'dynasor' package to predict observables from scattering experiments. We focus on our recent work on crystalline benzene as an example system, but the approach is readily extendable to other systems.

MM 17.4 Mon 18:30 Poster F

Interoperable data workflows: A case study on non-vdW 2D systems — •Mani Lokamani[1], Gregor Michalicek[2], Daniel Wortmann[2], Stefan Blügel[2], and Rico Friedrich[1,3,4] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [2]Forschungszentrum Jülich — [3]TU Dresden — [4]Duke University, Durham, USA

Interoperability and compatibility of research data and workflows from different, complementary simulation ecosystems are the key enabler for data-driven materials design. Two such simulation environments are (i) AFLOW [1], with its standardized workflows that generate huge amounts of compatible data, and (ii) AiiDA [2], which provides a customizable workflow that is often employed for dedicated projects by interfacing with several different *ab initio* programs.

Here, we aim at exploring the transferability and interoperability of data and workflows between the two frameworks. As a case study, we focus on the emerging class of non-van der Waals 2D materials, which have attracted considerable interest in recent years due to their unique electronic and magnetic properties [3]. In the first step, metadata are retrieved using AFLOW. Then, the extracted parameters are adapted with an AiiDA-plugin for accurate electronic structure calculations using the full-potential all-electron code FLEUR [4] within AiiDA.

We acknowledge support from the Helmholtz HIDA trainee network.

[1] C. Oses *et al.*, Comput. Mater. Sci. **217**, 111889 (2023).
[2] G. Pizzi *et al.*, Comput. Mater. Sci. **111**, 218 (2016).
[3] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).
[4] The FLEUR project: https://www.flapw.de.

MM 17.5 Mon 18:30 Poster F

Investigating phonons in superconducting Lanthanum Hydride using ab initio methods accelerated by machine learning potentials. — •Abhishek Raghav[1], Kousuke Nakano[2], and Michele Casula[1] — [1]Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, Paris, France — [2]Center for Basic Research on Materials, National Institute for Materials Science (NIMS), Tsukuba, Japan

Hydrogen rich materials with calthrate structures are an important class of superconducting materials. Lanthanum hydride (LaH_{10}) is one such material, demonstrated to show superconductivity at 250 K and 170 GPa.

Phonon spectrum and electron-phonon coupling are important ingredients used to predict superconductivity, being of BCS type. However, computing accurate phonons for hydrogen calthrate materials requires including anharmonicity due to nuclear quantum effects. In this work, we use the path integral molecular dynamics (PIMD) formalism to compute accurate anharmonic phonons. It is observed that, phonons for LaH_{10} ($Fm\bar{3}m$ phase), as predicted by PIMD are dynamically stable over the experimentally relevant pressure range, in contrast with the harmonic phonons. We also use the energies and forces computed during PIMD to train a machine learning potential (MLP) for LaH_{10} using operator quantum machine learning. This MLP is then used to drive simulations with larger supercells, to compute phonons efficiently and accurately.

MM 17.6 Mon 18:30 Poster F

Machine-learning based optimization of hafnium-zirconium oxide compositions for stable ferroelectric applications in non-volatile memories — •Arunima Singh and Patrick Rinke — Department of Applied Physics, Aalto University

CMOS-compatible hafnium dioxide (HfO_2) based ferroelectrics (FE) are widely studied for use in non-volatile memories. Zr-doping of HfO_2 i.e. hafnium-zirconium oxide (HZO) has further improved the FE properties. However, the optimum HZO structure and stoichiometry ($Hf_{1-x}Zr_xO_2$) still needs to be found. In this work, we used machine-learning assisted density-functional theory (DFT) calculations [1] to map out and characterize $Hf_{1-x}Zr_xO_2$ and to find optimal configurations in the materials space. We built an initial dataset of $Hf_{1-x}Zr_xO_2$

structures and their corresponding single point DFT energies. A kernel ridge regression (KRR) machine learning model is trained on this dataset and then further refined with active learning that picks appropriate structures from DFT relaxation trajectories. The atomic structures are represented in the vector form with many-body tensor representation (MBTR). With the refined KRR model, we explored the full HZO configuration space and optimized for structural stability and FE (also calculated with DFT).
[1] J. Laakso, M. Todorović, J. Li, G. X. Zhang & P. Rinke, *Compositional engineering of perovskites with machine learning*, Physical Review Materials, 6(11), 113801, (2022).

MM 17.7 Mon 18:30 Poster F

Computational Workflow for Defect Calculations for Solar Cell Applications — •Lotte Kortstee and Ivano Eligio Castelli — Department of Energy Conversion and Storage, Technical University of Denmark, Anker Engelundsvej 411, DK 2800 Kgs. Lyngby, Denmark

To aid the discovery of new functional materials and encourage the shift towards sustainable energy sources, the employment of computational tools is essential. A workflow-centered approach is used to study defects in perovskite materials that serve as an indicator for solar cell efficiency.

Using the framework of Density Functional Theory, a workflow is created using the Pydefect package and Atomistic Simulation Environment (ASE). The workflow is used to generate a chemical phase diagram, that identifies the chemical potentials under which the target material is stable. From there, defect calculations are performed on vacancies, interstitials and antisites of varying charge. Moreover, the band-structure and density of states of the compounds are determined to locate charge transition levels in relation to the band gap edges. Using Climbing Image Nudged Elastic Band (CINEB), the kinetics of point defects in the structure can be assessed and related to the formation energy of point defects.

We have applied this workflow to discover perovskites for solar cell applications, focusing on gold-containing tetragonal double perovskites. The properties of these materials are being investigated experimentally at our partner university.

MM 17.8 Mon 18:30 Poster F

Modification of bimetallic sulfide anodes for sodium ion storage — •Zidong Wang — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Due to their high specific capacity and long cycle life, bimetallic sulfides are the preferred choice of researchers as anodes in sodium-ion batteries (SIBs). However, studies indicate that this class of materials often requires expensive elements such as Co, Sb, Sn, etc., and their performance is insufficient with the use of inexpensive Fe, V alone. Therefore, there is a need to explore the relationship between metal cations and anode performance so that the requirements of cost reduction and performance enhancement can be met simultaneously. In this work, a series of partially re-placed sulfides with different cation ratios have been prepared by hydrothermal method followed by heat treatment. By partially replacing Co in NiCo sulfides, all samples show improved capacity and stability over the original NiCo sulfides. As a result, the metal elements have different oxidation states, which leads to a higher capacity through their synergistic effects on each other.

MM 17.9 Mon 18:30 Poster F

Machine-Learned Molecular Dynamics Simulations of Doping Effects in Sodium Ion Conductors — •Namita Krishnan, Takeru Miyagawa, Manuel Grumet, Waldemar Kaiser, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany

Na-based solid-state ion conductors (SSICs) are set to revolutionize next-generation batteries due to low cost and availability relative to their lithium-based counterparts. Still, Na-based SSICs have considerably lower ionic conductivities relative to conventional electrolytes, a factor that hampers their commercialization. Doping is one way to mitigate this disadvantage by maximizing ion conduction pathways without compromising the host lattice's structural integrity [1,2]. A sophisticated choice of dopant elements requires a deep understanding of the interplay between the dopants, mobile Na ions, and the host lattice. Ab initio molecular dynamics (AIMD) simulations offer atomistic insights into the lattice dynamics of doped SSICs but are computationally tedious. Therefore, we investigate the accuracy of machine-learned molecular dynamics (MLMD) for vibrational properties and diffusion coefficients of doped sodium ion conductors compared to AIMD simulations. We then apply the ML-generated force fields to investigate the effect of homovalent and aliovalent doping in Na_3SbS_4.

References [1] T. Fuchs, et al. ACS Energy Lett., 2019, 5, 1, 146-151. [2] R. Jalem, et al. J. Mater. Chem. A, 2022 10, 5, 2235-2248.

MM 17.10 Mon 18:30 Poster F

Disorder in electronic properties of 2D and 3D perovskites on the nanoscale — •Andrii Shcherbakov[1,2], Darwin Korte[1], Shangpu Liu[1,2], Markus Heindl[1,2], Stanislav Bodnar[1,2], Jonathan Zerhoch[1,2], and Felix Deschler[1] — [1]Physikalisch-Chemisches Institut Universität Heidelberg, Im Neuenheimer Feld 229, D-69120 Heidelberg — [2]Walter Schottky Institut Technische Universität München,Am Coulombwall 4, 85748 Garching bei München

Because of outstanding semiconducting properties like high quantum yield, tuneability, and potential to form quantum confined systems, organic-inorganic hybrid perovskites have proved themselves as attractive candidates for various optoelectronic applications, including efficient photodetectors, light emitting diodes and solar cells. Local electronic properties affected by the disorder caused by strain, defects, and differences in confinement have a direct influence on the optical properties and the device's performance. By studying the types of such inhomogeneities, their influence on key semiconducting properties, and their dependence on the fabrication process, we can adjust the latter to achieve the best performances. Here, we start investigating our test materials with the means of confocal (circular) photoluminescence spectroscopy, allowing to study disorder on the microscale. By further employing nearfield nanoscopy, we achieve spatially resolved material response with a resolution below the diffraction limit. Finally, we find a correlation between the fabrication conditions and the disorder, suggesting us ways of increasing the performance of the product material.

MM 17.11 Mon 18:30 Poster F

Functional properties of aerosol deposited thick lead-free piezoelectric ceramic films — •Michel Kuhfuss[1], Juliana G. Maier[1], Alexander Martin[2], Ken-ichi Kakimoto[2], Neamul H. Khansur[1], and Kyle G. Webber[1] — [1]Department of Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany — [2]Department of Life Science and Applied Chemistry, Nagoya Institute of Technology, Nagoya, Japan

The powder aerosol deposition (AD) method is a technique to deposit thick, dense ceramic films through room temperature impact consolidation (RTIC). AD is a promising method for applications such as piezoelectric energy harvesting due to being cost-effective and rapid. However, deposited films differ from bulk ceramics due to internal stress, RTIC-induced defects, and nanometer-range grain size. Therefore, the impact on the functional properties of different lead-free piezoelectric materials is investigated with electromechanical measurements. They reveal a direct connection between the piezoelectric response and the grain size. For comparison, the grain size dependence is analyzed with in situ electric field-dependent synchrotron X-ray diffraction. Further, processing methods such as annealing are conducted to enhance the properties of the deposited films.

MM 17.12 Mon 18:30 Poster F

interaction of hydrogen with local heterogeneities: correlating simulations and experiments — •Onur Can Şen[1,2,3], Santiago Benito[2], Sebastian Weber[2], and Rebecca Janisch[3] — [1]IMPRS SusMet, Max-Planck-Institut für Eisenforschung GmbH — [2]LWT, Ruhr-Universität Bochum — [3]ICAMS, Ruhr-Universität Bochum

The term "hydrogen embrittlement" (HE) refers to multiple phenomena related to the detrimental effects of hydrogen in metallic materials. The most effective approach to mitigate HE involves reducing hydrogen diffusion within microstructures, requiring a thorough understanding of the impact of local heterogeneities at various length scales. Advanced experimental and computational methods exist for this purpose, but they are usually applied to samples or models, of rather different complexity, and thus it is always a question of how to compare and combine their results. In this study, ab initio density functional theory calculations were used to calculate the diffusion barrier of hydrogen under the influence of different local chemistry. Simultaneously, differently alloyed Fe-based alloys are produced on a laboratory scale, and subjected to various heat treatments to achieve microstructures representing different local microstructural character-

istics, for which atomistic simulation models shall be set up as well. This poster shows the first insights on how to combine more effectively simulation and experimental methods to shed light on how inevitable heterogeneities impact the hydrogen behavior in iron and steel.

MM 17.13 Mon 18:30 Poster F

Mechanochemical Pathway to Nickel — •Jikai Ye[1], Christian H. Liebscher[2], and Michael Felderhoff[1] — [1]Max-Planck-Institut für Kohlenforschung, Department of Heterogeneous Catalysis, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Metal oxide reduction is the key step to metal production in the process of both primary and secondary metal production. However, traditional methods usually correlate with high energy consumption from heating and CO_2 emission from carbonaceous reductants. Mechanochemistry describes certain reactions that can happen with the help of mechanical forces under much milder conditions, which could enable more sustainable pathways for metal productions. In this work, the possibility of reducing metal oxides at room temperature under hydrogen with ball-milling is confirmed, using NiO as an example. In a planetary ball-mill batch system under hydrogen pressure, NiO could be partially reduced, reaching an equilibrium state upon generation of water vapor. Further, with the help of a home-built gas-flow shaker-mill system, generated water from the reaction between NiO and hydrogen could be removed continuously. A much higher reduction degree could therefore be achieved. With mild heating (<100 °C) during milling, reaction rate could be significantly increased benefiting from faster desorption of water. With this method, Ni nanoparticles were synthesized. Primitive tests also confirm that the as-synthesized Ni nanoparticles exhibit high catalytic activity over hydrogenation.

MM 17.14 Mon 18:30 Poster F

Raman Spectroscopy and Photoluminescence Studies on Recyclate-based MgO-C Composites — •Julia Richter[1], Cameliu Himcinschi[1], Mahnaz Mehdizadehlima[2], Serhii Yaroshevskyi[3], Till Manon Jannis Stadtmüller[3], and Jens Kortus[1] — [1]Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Straße 23, D-09599 Freiberg, Germany — [2]Institute of Materials Science, TU Bergakademie Freiberg, Gustav-Zeuner-Straße 5, D-09599 Freiberg, Germany — [3]Institute of Ceramics, Refractories and Composites, TU Bergakademie Freiberg, Agricolastraße 17, D-09599 Freiberg, Germany

Re-usage, recycling and upcycling of MgO-C refractories are crucial for resource efficiency. Antioxidants used as additives as well as metal and slag residuals reduce the quality of the recycled raw material. Environmentally friendly binders, e.g. lignin-collagen systems, are supposed to replace commonly used binders, such as pitch and resin, in order to save resources and to lower CO2 emissions as well as harmful effects on the environment. In this work, Raman and photoluminescence (PL) spectroscopy as sensitive, non-destructive, non-contact methods are applied to detect impurities and to characterize the carbon structures, in particular carbon cluster size, depending on the binder system in the refractory material.

On the other hand, MgO-C recyclate-based anode materials for application in the extraction of aluminum by fused-salt electrolysis are investigated by Raman and PL and their spectra compared with those of pure materials.

MM 17.15 Mon 18:30 Poster F

Optothermal analysis of Indium thiospinels — •André Strassheim[1], Cameliu Himcinschi[1], Ayberk Özden[2], Esteban Zuñiga-Puelles[3], Roman Gumeniuk[3], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09599 Freiberg, Germany — [2]TU Bergakademie Freiberg, Institute of Electronic and Sensor Materials, D-09599 Freiberg, Germany — [3]TU Bergakademie Freiberg, Institute of Experimental Physics, D-09599 Freiberg, Germany

The temperature dependence of thermal conductivities of crystalline Indium thiospinels were characterized by optothermal Raman spectroscopy, a contactless method that can be used for small sample volumes. The obtained values are in fair agreement with those obtained from conventional laser flash analysis and thus, validates the employed technique. The temperature-dependent thermal conductivity of one Indium thiospinel sample was measured from 100 K to 343 K in steps of 50 K and ranged from 5.1 $\frac{W}{mK}$ to 1.7 $\frac{W}{mK}$.

Furthermore, a reversible β ($I4_1/amd$) to α ($Fd\bar{3}m$) phase transition was identified through temperature-dependent Raman spectroscopy. It was observed to be reversible and to occur between 440 K and 450 K.

In conclusion, this study suggests that optothermal Raman spectroscopy emerges as a valuable technique for probing the thermal properties of materials, particularly in cases where material volume is limited and when dealing with arbitrary shapes.

MM 17.16 Mon 18:30 Poster F

Direct visualization of electric current induced dipoles of atomic impurities — •Yaowu Liu[1,2], Zichun Zhang[1], Sidan Chen[1], Shengnan Xu[1], Lichen Ji[1], Wei Chen[1], Xinyu Zhou[1], Jiaxin Luo[1], Xiaopeng Hu[1], Wenhui Duan[1], Xi Chen[1], Qikun Xue[1,3,4,5], and Shuaihua Ji[1,5] — [1]State Key Laboratory of Low-Dimensional Quantum Physics, Department of physics, Tsinghua University, Beijing 100084, China — [2]Center for Quantum Nanoscience, (IBS), Seoul 30760, Republic of Korea — [3]Beijing Academy of Quantum Information Sciences, Beijing 100193, China — [4]Department of Physics, Southern University of Science and Technology, Shenzhen 518055, China — [5]Frontier Science Center for Quantum Information, Beijing 100084, China

Learning electron scattering around atomic impurities is vital for comprehending the basic electronic transport phenomena. Despite many efforts in the past several decades, atomic scale transport around single point-like impurities has yet been achieved. Here, we report the direct visualization of the electric current induced dipoles around single atomic impurities in epitaxial bilayer graphene [arXiv:2309.01182]. We find the directions of these dipoles are determined by the charge polarity of the impurities, revealing the direct evidence for the existence of the carrier density modulation effect proposed by Landauer in 1976 [Phys.Rev.B 14,1474 (1976)]. Furthermore, by in situ tuning local current directions, these dipoles are redirected correspondingly. Our work paves the way to explore the quantum transport phenomena at single atomic impurity level.

MM 17.17 Mon 18:30 Poster F

Tuning thermal and ionic transport properties of sodium superionic conductors for advanced energy storage: insights from molecular dynamics simulations — •Insa de Vries, Freya Hallfarth, and Nikos Doltsinis — Institute of Solid State Theory, University of Münster, Wilhelm-Klemm-Straße 10, 48149 Münster

In the pursuit of resource-efficient and sustainable energy storage solutions, sodium-based electrolytes increasingly attract attention as a compelling choice for energy materials. Notably, sodium superionic conductor (NASICON)-type lattices have demonstrated promising ionic conductivities, positioning them as viable candidates for battery applications [1]. However, the development of a secure battery design necessitates, in addition, a comprehensive understanding of thermal conduction properties to mitigate localized heat accumulation during battery operation.
We conducted classical molecular dynamics simulations of the $Na_{1+x}Zr_2Si_xP_{3-x}O_{12}$ class of compounds for various stoichiometries (x=2, 2.4, and 2.8) using an interionic potential derived before [2]. Structural order of the Si and P cations is found to enhance diffusion. Its influence on thermal conductivity, assessed by a Green-Kubo approach, is discussed. A decrease in thermal conductivity is observed upon suppression of sodium ion diffusion.

[1] C. Zhao et al., Adv. Energy Mater. 2018, 8, 1703012
[2] P. Kumar & S. Yashonath, J. Am. Chem. Soc. 2002, 124, 3828

MM 17.18 Mon 18:30 Poster F

Ab-initio simulation of electronic transport in amorphous phase change materials — •Nils Holle[1], Sebastian Walfort[1], Riccardo Mazzarello[2], and Martin Salinga[1] — [1]University of Münster, Institute of Materials Physics, 48149 Münster — [2]Sapienza Università di Roma, Department of Physics, I-00185 Roma

As the global demand for computing resources continues to grow, the need to improve the energy efficiency of computing hardware is becoming increasingly important. The miniaturisation of electronic devices based on phase change materials (PCMs) has been shown to enable significant reductions in power consumption. These materials exist in both a crystalline and an amorphous configuration and exhibit a strong electrical contrast between these configurations. This makes them interesting for a wide range of applications, such as data storage and neuromorphic computing. A detailed understanding of electronic transport is a crucial step towards designing a new generation of energy-efficient functional electronic devices. However, de-

spite many years of research, electronic transport in amorphous PCMs is still not fully understood, as it is complicated by disorder and its consequences, such as structural inhomogeneity. We study transport in a single-element PCM that is strongly confined between adjacent electrodes. The combination of density functional theory and non-equilibrium Green's functions provides the ideal means to gain ab-initio insight into electronic structure and transport on an atomistic scale. Based on our observations, we propose a new physical picture where conductivity is governed by local variations in Peierls-like distortions.

MM 17.19 Mon 18:30 Poster F

Accurate ab initio vacancy properties in concentrated Mo-Ta alloys from machine-learning potentials — •Xiang Xu[1,3], Xi Zhang[1], Sergiy Divinski[2], and Blazej Grabowski[1] — [1]Institute for Materials Science, University of Stuttgart, Germany — [2]Institute for Materials Physics, University of Münster, Germany — [3]Institute for Materials Testing, Materials Science and Strength of Materials, University of Stuttgart, Germany

We utilize a bespoke machine-learning interatomic potential, i.e., moment tensor potential (MTP) to predict thermodynamic properties of vacancy formation. The highly optimized MTP is trained with snapshots from ab initio molecular dynamics simulations within the active learning framework. For the vacancy formation energy, we utilize the special quasi-random structure approach in conjunction with a statistical analysis, from which temperature-dependent formation Gibbs energies as well as averaged atomic environments can be extracted. We show that the temperature-dependent vacancy formation Gibbs energy due to "configurational excitations" has a negative entropy contribution while thermal vibrations provide a positive entropy. The local chemical environment effect and general trends are also analyzed.

MM 17.20 Mon 18:30 Poster F

Machine learning approach to obtaining the scattering self-energy from transmission calculations — •Fabian Engelke, Markus Kremer, Michael Czerner, and Christian Heiliger — Justus-Liebig-Universität, Institute for Theoretical Physics, Gießen, Germany

Aiming to assist the development of nanoscale electronic devices, we contribute to developing ab initio transport calculations. This work is particularly concerned with treating phase-breaking scattering events due to the electron-phonon interaction. In the Keldysh formulation of the non-equilibrium Green*s function formalism, as implemented in a Korringa-Kohn-Rostoker electronic structure code, those scattering events are characterized by an additional self-energy. Even though it is possible to estimate the self-energy, those calculations involve many approximations, such as k-vector averaging and Wannier-function interpolation of band structures.

Introducing a new way to calculate the self-energy, we train a deep neural network based on conventionally calculated self-energies and transmission calculation results from the Keldysh formulation. We then use this neural network to map transmission results based on the molecular dynamics Landauer approach back to the self-energy.

MM 17.21 Mon 18:30 Poster F

Multi-scale modeling of heat conduction in filled polymer composites — •Oliver Roser[1,2], Andreas Griesinger[3], and Othmar Marti[2] — [1]Center for Heat Management (ZFW), Stuttgart — [2]Institute of Experimental Physics, Ulm University — [3]Baden-Wuerttemberg Cooperative State University (DHBW), Stuttgart

When polymers are modified with granular fillers to increase thermal conductivity, the simultaneous viscosity increase of the composite often limits the allowable filler concentration and thus the achievable thermal conductivity. If fillers from several size classes are smartly combined, the viscosity increase can be mediated and the allowable filler concentration increased. The result is a complex material whose microstructure extends over several orders of magnitude. The largest particles used may be thousands of times larger than the smallest. For a detailed simulative analysis of the heat transport phenomena in such materials, we have designed a new multi-step homogenization approach. This approach allows us to take into account the filler structure in all size scales and to calculate the achievable thermal conductivity as a function of the filler composition. Starting with the heat transfer from the smallest filler particles into the polymer up to the large spatial heat paths between the largest filler particles, all effects are taken into account. We present our multi-step homogenization approach, experimental validation, and the results of computational studies on the optimal composition of filler blends.