FM 22: Focus Session: Materials Discovery III – New materials and functionalities by general principles

chairs: Hiroki Taniguchi (Nagoya University, JP), Akitoshi Nakano (Nagoya University, JP)

Discovering new functional materials is crucial to advance today's technologies, ranging from caloric cooling via catalysis to next-generation energy conversion and storage, such as thermoelectric, ferroelectric, and ionic conductor materials. New materials also form the basis for potential applications in quantum information technologies. This session provides a platform to highlight functional materials discoveries and how they come about. Notably, systematic searches with high-throughput synthesis approaches, as well as predictions from materials informatics, have helped to go beyond serendipitous discoveries in recent years. However, intuition guided by general principles remains an important factor. In this session, we particularly welcome contributions that showcase the discovery of new functional materials with original approaches. Diverse material systems - from well-established to emerging and niche classes across condensed-matter and materials physics - will be featured. Bringing together diverse discoveries in a single session will help delineate general principles and inspire future work.

Time: Friday 9:30–12:45 Location: BEY/0138

Invited Talk FM 22.1 Fri 9:30 BEY/0138

Topological thermoelectrics for solid state cooling — •Yu Pan[1] and Claudia Felser[2] — [1]Chongqing University, Chongqing, China — [2]Max Planck Institute for Chemical Physics of Solids

Thermoelectric effects enable the direct conversion between thermal energy and electrical energy, and has broad application potential in areas such as thermoelectric power generation, solid-state cooling, and precise temperature control. Classic thermoelectric materials mainly focus on heavily doped narrow bandgap semiconductor materials, whose thermoelectric performance is limited above room temperature (> 300 K). So far, further enhancement of thermoelectric performance at low temperatures (<300 K) faces significant challenges, severely restricting the application of thermoelectric materials in low-temperature solid-state cooling. In recent years, the surge of topological quantum materials has triggered many novel thermoelectric transport behaviors, especially the significantly enhanced low-temperature thermoelectric performance under magnetic fields, providing new opportunities to greatly improve low-temperature thermoelectric performance. For example, their linear-dispersion energy band structures and ultrahigh mobility significantly enhance the magneto-Seebeck effect and Nernst effect. On the other hand, topological quantum materials with broken symmetry can exhibit an anomalous Nernst thermoelectric potential far higher than that of conventional ferromagnets due to the presence of nonzero Berry curvature, laying a scientific foundation for thermoelectric applications of the anomalous Nernst effect under low or even zero magnetic fields.

FM 22.2 Fri 10:00 BEY/0138

Topological quantum materials for high performance heterogenous catalysis — •Xia Wang and Claudia Felser — Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

The electronic structure of a catalyst plays a pivotal role in governing its performance1. Topological quantum materials, known for their symmetry-protected electronic states, offer a unique platform to bridge solid-state topology and heterogeneous catalysis. When combined with chirality, topological quantum materials give rise to novel material systems exhibiting distinct chiral phenomena, opening new avenues for the development of next-generation chiral catalysts. Situated at the interface of condensed matter physics and chemistry, the emerging field of topological catalysis exploits the exotic quantum properties of topological quantum materials to not only enhance catalytic activity and selectivity but also to enable fundamental studies of reaction mechanisms. Our recent experimental and theoretical work demonstrates a direct link between spin-orbit coupling and the kinetics of oxygen electrocatalysis, including both the oxygen reduction and evolution reactions. Furthermore, we show that external stimuli such as magnetic fields can effectively tune catalytic performance by modifying the topological features of the electronic structure. Together, these insights establish topological quantum materials as a compelling framework for designing high-performance, field-tunable catalysts, with far-reaching implications for asymmetric synthesis to probing the origins of life.

FM 22.3 Fri 10:15 BEY/0138

Ta2PdSe6: A guide towards high performance thermoelectric semimetals — •Akitoshi Nakano — Nagoya University, Nagoya, Japan

We have recently discovered that a transition-metal chalcogenide Ta2PdSe6 exhibits an extraordinary thermoelectric property despite its semimetal character. Ta2PdSe6 crystallizes in a layered structure, each layer of which consists of quasi-one-dimensional chains formed by prismatic TaSe6 and square-planner PdSe4. The thermoelectric property measured along this direction is highly exotic; an ultra-high conductivity (σ) above 10^6 Ω^-1cm^-1 is compatible with a substantial thermopower (S) of 40 μVK^-1 at 20K. As a result, the power factor (= S^2σ) reaches above 2000 μWcmK^-2, which is top level among bulk thermoelectric materials thus far.

Furthermore, we have found that the thermal conductivity of Ta2PdSe6 is relatively small (~ 100 Wm^-1K^-1) for such a good electrical conductor associated with a serious violation of the Wiedemann-Franz law. As a result, the thermoelectric figure of merit Z (= S^2$\sigma\kappa$^-1) of Ta2PdSe6 at 14 K reaches as high as 3*10^-3 (K^-1), which is comparable to Bi2Te3 at 300 K.

In the presentation, we will discuss the origin of the anomalous transport properties of Ta2PdSe6 from the viewpoint of the carrier dynamics.

FM 22.4 Fri 10:30 BEY/0138

Symmetry-Driven Transitions Between Flat Bands and Dirac Cones in Bilayer Kagome Lattices — •Taylan Gorkan — Bilkent University-UNAM

Flat bands (FBs) and Dirac cones represent two distinctive features of topological electronic systems, yet a unified mechanism enabling transitions between them has remained elusive to date. Here, we demonstrate a symmetry-governed and tunable transition from flat bands to Dirac cones in AB-stacked bilayer kagome lattices. This transition is mediated by the interplay between destructive quantum interference (DQI), C3 rotational symmetry, and spatial inversion symmetry. Strong interlayer coupling enhances DQI and stabilizes compact localized states that produce FBs, while weaker coupling allows C3 and inversion symmetries to dominate, giving rise to robust Dirac nodal points. Using a minimal tight-binding model, we map the continuous evolution of topological states-including type-II and type-III Dirac cones, spin-1 Dirac nodes, and partial flat bands-as a function of interlayer coupling. We further demonstrate this transition mechanism by examining an AB-stacked bilayer derived from the experimentally synthesized Nb3TeCl7 structure. In particular, first-principles calculations on bilayer Nb3TeCl7 reveal that vertical strain/pressure modulates interlayer interactions, enabling the entire FB-Dirac cones transition sequence. These findings establish a realistic novel pathway for gaining further insights into flat-band physics and engineering tunable topological phases in two-dimensional materials.

FM 22.5 Fri 10:45 BEY/0138

Emergent High Conductivity Transport Channel in $Bi_{12}Rh_3Ag_6I_9$ Single-Crystalline Multilayer Heterostructure — •Nicolas Perez[1], Eduardo Carrillo-Aravena[2], Christian Niclaas Saggau[1], Kornelius Nielsch[1], and Michael Ruck[2] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01062

Dresden, Germany

$Bi_{14}Rh_3I_9$-type weak 3D topological insulators (TIs) can be seen as nano-periodic multilayer heterostructures of 2D TIs spaced by topologically trivial insulators. The newest member $Bi_{12}Rh_3Ag_6I_9$ exhibits 2D cationic conductivity in the silver iodide spacer, which allows to electrochemically adjust the Fermi level, and has the widest band gap so far in this family of compounds, 286 meV. It shows strongly increasing diamagnetism at low temperatures in a field perpendicular to the layers. Magnetoresistance measurements in macroscopic crystals reveal confinement and oscillatory behaviour, which coincides with a drastic drop in resistivity both parallel and across the layers. The observation of such an effect in a crystalline multilayer structure is compatible with the theoretically predicted formation of a collective [1+1]-dimensional sheath state involving all lateral crystal faces and probably arising from tunneling between the protected edge states of the numerous closely spaced 2D TI layers. A macroscopic system of some 10^5 coupled spin channels appears promising for applications in spintronics and quantum computation.

FM 22.6 Fri 11:00 BEY/0138

Simulating the Schrödinger equation in anti-Hermitian electrical circuits — •Ivan Scolan[1], Ronny Thomale[2], Jasper Van Wezel[3], Viktor Könye[3], Ali Moghaddam[4], Jeroen Van Den Brink[1], and Joseph Dufouleur[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden — [2]Institute for Theoretical Physics and Astrophysics, University of Würzburg — [3]Institute for Theoretical Physics Amsterdam — [4]Faculty of Engineering and Natural Sciences, Tampere Finland

In recent years, a number of condensed matter lattice models have been realized using classical electric circuits, exploring topological phases hitherto inaccessible experimentally. In these previous works, the Hamiltonian of a system was implemented in a topo-electronic circuit, thus possessing the same spectrum as any equivalent condensed matter system, but the dynamics of the electronic circuit remained distinct from the quantum dynamics given by the Schrödinger equation. Here we propose a new way to realize electronic circuits that are equivalent to solid-state lattices based on anti-hermitian circuits the dynamic of which perfectly follows the Schrödinger dynamics.

Intrinsic symmetries of these circuits allow the experimental measurement of all eigenstates. Using this framework, we apply it to a 1D atomic chain with position-dependent hopping terms and experimentally retrieve the theoretical results presented in Mertens et al. (2022), Morice et al. (2021). Finally, we show how our method can be used to develop novel electronics which can be used for concrete applications and also for solving fundamental physics problems.

Coffee Break

FM 22.7 Fri 11:30 BEY/0138

Photo-dielectric synaptic plasticity in Zn-substituted $BaAl_2O_4$ — •Hiroki Taniguchi — Department of Physics, Nagoya University, Nagoya 464-8602, Japan

Optical control of material properties is pivotal for advancing the evolution from conventional electronics to next-generation photoelectronics. Although a variety of photo-induced phenomena, including the photovoltaic effect and photoconduction, have been well established as key mechanisms for photoelectronic devices, the optical manipulation of dielectric responses has remained comparatively unexplored.

Here, I demonstrate a photo-dielectric effect in partially Zn-substituted $BaAl_2O_4$, in which the dielectric permittivity increases under below-bandgap photo-irradiation without inducing photoconduction. First-principles calculations indicate that Zn substitution creates a unique defect complex. Upon photo-irradiation, photo-generated electron*hole pairs form a local dipole around this defect complex, producing an additional polarization contribution and consequently enhancing the dielectric permittivity. Furthermore, transient permittivity measurements under sequential pulsed optical excitation reveal synaptic-plasticity-like responses in Zn:$BaAl_2O_4$, highlighting its potential for neuromorphic device applications.

FM 22.8 Fri 11:45 BEY/0138

Triclinic distortion in titanite-type oxides CaSnGeO5 and SrSnGeO5 — •Taro Kuwano[1], Hiroko Yokota[1], Manabu Hagiwara[2], Toshiya Uohashi[3], Akitoshi Nakano[3], and Hiroki Taniguchi[3] — [1]4259 Nagatsuta-cho, Midori-ku, Yokohama, Kanagawa, 226-8501 Japan — [2]3-14-1 Hiyoshi, Kohoku-ku, Yokohama, Kanagawa, 223-8522 Japan — [3]Furo-cho, Chikusa-ku, Nagoya, Aichi, 464-8602 Japan

Titanite-family oxides have been emerging as a novel vein of antiferroelectric materials owing to their unique pseudo-one-dimensional structure hosting "antipolar arrangement of polar chains." In this study, we focus on another characteristic feature of the titanite-type structure: ferroelastic phase transition associated with triclinic distortion. We will propose one couple of representatives, SrSnGeO5 and CaSnGeO5, which exhibit the phase transition at about 150 and 600 K, repectively. In comparison with the cases of SrZrGeO5 and CaZrGeO5, the origin of the triclinc distortion will be discussed.

FM 22.9 Fri 12:00 BEY/0138

Interplay between Lattice Dynamics and Free Electrons in Polar Metals: A Chemical-Bonding Perspective — •Hiroto Kikuchi[1], Suguru Yoshida[1], Hiroshi Takatsu[1], Kantaro Murayama[1], Peter Lemmens[2], and Hiroshi Kageyama[1] — [1]Department of Energy and Hydrocarbon Chemistry, Graduate School of Engineering, Kyoto University, Nishikyo-ku, Kyoto 615-8510, Japan — [2]Institute for Condensed Matter Physics, Technische Universitat Braunschweig; Braunschweig 38106, Germany

Polar-nonpolar (P-NP) transitions in metals such as $LiOsO_3$ show that polar order can coexist with metallicity, defining "polar metals" as a new class of quantum materials. However, the microscopic mechanism remains under debate, with competing scenarios invoking electron-phonon coupling and coordination bonding.

We recently found that metallic $LiReO_3$, isostructural with $LiOsO_3$ and adopting the $LiNbO_3$-type structure, undergoes a P-NP structural transition at T_s = 170 K. Unlike the second-order transition in $LiOsO_3$, $LiReO_3$ shows thermal hysteresis and strong lattice softening, indicating enhanced fluctuations between polar and nonpolar phases.

We investigated Raman scattering across T_s, combined with phonon calculations and crystal orbital Hamilton population (COHP) analysis, and reveals strongly redshifted LiO_6-related optical phonons in $LiReO_3$ compared with $LiOsO_3$. These results, supported by computed force constants and bond strengths, provide a unified picture of phonon softening and polar stability in metallic $LiReO_3$.

FM 22.10 Fri 12:15 BEY/0138

NaSICON with Mg and Ca as charge carriers — •Katharina Helmbrecht and Axel Gross — Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany

While the Mo_6S_8 chevrel phase is frequently used as cathode material in Mg–ion batteries, theoretical studies on this material are comparatively scarce. Mo_6S_8 as a cathode material for mono– and multivalent–ion batteries is an interesting candidate. Furthermore, magnesium and calcium both show much promise a charge carriers for a suitable battery system of the future.

In this work we study the behavior of mono– and multi–valent charge carriers (Li, Na, K, Mg, Ca, Zn, Al) at the low vacancy limit of intercalation and its influence on stability and kinetics of Mo_6S_8 intercalation compounds to reach fundamental understanding of the material and its properties.

Upon varying the charge carriers in the Chevrel phase at the upper vacancy limit in a previous study [1], their diffusion barriers were observed to scale linearly with the ion size, almost independent of the charge of the considered ions. This indicates a rather unique and geometry dominated diffusion mechanism in the chevrel phase and raises the question whether this trend persists at the lower vacancy limit.

[1] K. Helmbrecht, H. Euchner, A. Groß, Batteries Supercaps **5**, e202200002 (2022).

FM 22.11 Fri 12:30 BEY/0138

High pressure crystallography: from mineral physics to material sciences — •Leonid Dubrovinsky — BGI, Bayreuth University, Bayreuth, Germany

Modern science and technology rely on the fundamental knowledge of matter that is provided by crystallographic studies. About a decade ago, our group pioneered an approach to the SCXRD data collection and analysis for the products of chemical reactions in laser heated DACs. Since then we have designed and built new instrumentation to enable sophisticated in situ experiments in house and on synchrotron radiation facilities. Our efforts have pushed the range of static pressures achievable in a DAC up to 1 TPa and enabled single-crystal X-ray diffraction experiments at such extreme conditions. Structural studies at simultaneous high pressures of over ~200 GPa and temperatures of

several thousand degrees have also become possible. This has led to remarkable findings in solid state physics, mineral physics, and chemistry at extreme conditions.We illustrate application of new methodology for simultaneous high-pressure and high-temperature single crystal diffraction studies using examples of investigations of chemical and phase relations in the halides, nitrides, and carbonates.