# FM 9: Focus Session: Materials Discovery II – High throughput searches for functional magnetic materials (joint session FM/MA)

chairs: Jan Schultheiß (Norwegian University of Science and Technology, NO), Hiroki Taniguchi (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: Tuesday 14:00–15:30 Location: BEY/0138

**Invited Talk** FM 9.1 Tue 14:00 BEY/0138

**Thin film combinatorial studies of functional magnetic materials** — •Nora Dempsey — Institut NEEL, CNRS/UGA, Grenoble, France

Combinatorial studies based on the preparation and characterisation of compositionally graded thin films are being used for the screening and optimization of a range of functional materials [1]. When combined with Machine Learning (ML), such high-throughput film-based studies hold much potential to guide data driven design of new materials [2,3]. In this talk I will outline our work at Institut Néel on high throughput fabrication and characterisation of functional magnetic materials as well as our recent developments concerning data handling and analysis. I will then show examples from on-going studies of the effect of composition and fabrication conditions on both structural and magnetic properties of hard magnetic and magnetocaloric materials. I will finish up by briefly outlining preliminary results from ML-driven data analysis for the accelerated development of functional magnetic materials with reduced dependence on critical elements, carried out in the framework of various collaborations. [1] ML Green et al., J. Appl. Phys. 113 (2013) 231101 [2] A.G. Kusne et al. Sci. Rep. 4 (2014) 6367 [3] A. Ludwig, npj Comput. Mater. 5 (2019) 70

FM 9.2 Tue 14:30 BEY/0138

**Potentially magnetic platinum oxides obtained by computationally guided high-pressure synthesis** — •Yasuhito Kobayashi[1], Akitoshi Nakano[2], Shunsuke Kitou[3], Tomasz Klimczuk[4], Hidefumi Takahashi[1,5], and Shintaro Ishiwata[1,5] — [1]Division of Materials Physics, The University of Osaka, Japan — [2]Department of Physics, Nagoya University, Japan — [3]Department of Advanced Materials Science, The University of Tokyo, Japan — [4]Advanced Materials Center, Gdansk University of Technology, Poland — [5]Institute for Open and Transdisciplinary Research Initiatives, The University of Osaka, Japan

The exploration of Pt-based oxides has remained significantly limited, primarily due to the high chemical inertness of platinum and the typically nonmagnetic $d^6$ or $d^8$ electronic configurations. Here, we report the discovery of a new layered homologous series of Pt-based ternary oxides, $Na(PtO_2)_{2n+1}$ ($n$ = 1, 2), synthesized through a combination of highly oxidizing high-pressure techniques and density functional theory (DFT) calculations. This series features unprecedented layered structural motifs composed of rutile-based $PtO_6$ octahedra and one-dimensional $PtO_4$ square-planar chains, distinct from the perovskite-based Ruddlesden-Popper oxides. We discuss the possibility that this layered homologous series represents the first realization of a magnetic Mott insulator within Pt-based oxides, where $NaPt_3O_6$ ($n$ = 1) exhibits localized spin behavior with an effective spin $S$ = 1/2, likely arising from the unusual $d^7$ electronic configuration of square-planar $Pt^{3+}$ along with one-dimensional antiferromagnetic interactions.

FM 9.3 Tue 14:45 BEY/0138

**Magnetism and electrical and thermal transport in the natural $Fe_{1-x}Mn_xWO_4$ ($x$=0.2) mineral from Potosí, Bolivia** — •Skachko Dmytro[1], Bohdan Kundys[2], Volodymyr Levytskyi[1], Esteban Zuñiga-Puelles[1], Andreas Leithe-Jasper[3], and Roman Gumeniuk[1] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [2]Université de Strasbourg, CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, Strasbourg F-67000, France — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

The natural ferberite single crystal of $Fe_{0.8}Mn_{0.2}WO_4$ composition with the monoclinic $NiWO_4$-type structure ($P2/c$) [$a$ = 4.74751(6) Å, $b$ = 5.71335(7) Å, $c$ = 4.96847(5) Å, $\beta$ = 90.15(1)°] reveals multiple magnetic transitions at $T_{N1}$ = 67(1) K, $T_{N2}$ = 28(3) K, $T_{N1}^{cp}$ = 66(1) K and $T_{N2}^{cp}$ = 8(1) K. The reduced magnetic entropy of ≈ $R$ln3 observed near $T_{N1}$ indicates the simplified $LS$-coupling scheme to fail in the description of complex magnetic behavior of the studied ferberite. The temperature dependence of electrical resistivity [$\rho(T)$] shows a semiconducting exponential decay saturating at ≈ 300 K. The activation energy of the decay is found to be ≈310 meV. Temperature dependence of thermal conductivity [$\kappa(T)$] is characterized by a well defined maximum at ≈68 K, which is described by the Debye-Callaway model, pointing to the dominance of phonon scattering on defects and *umklapp* processes. Despite revealing relatively low $\kappa(T)$ and high Seebeck coefficient $Fe_{0.8}Mn_{0.2}WO_4$ is rather poor thermoelectric material because of enhanced $\rho(T)$.

FM 9.4 Tue 15:00 BEY/0138

**Ab initio-based phase diagrams for compositionally complex ThMn12-type alloys** — •Sourabh Kumar[1], Semih Ener[2], and Tilmann Hickel[1] — [1]Bundesanstalt für Materialforschung und -prüfung, 12489 Berlin — [2]Technische Universität Darmstadt, 64289 Darmstadt

The structural and chemical stability of rare-earth-based transition-metal (such as Nb, Ce, and Sm) alloys is critical in determining the performance of modern hard magnets (HMs), particularly their coercivity and thermal robustness. This study examines the intrinsic phase competition in (Sm/Ce)-(Fe/Co)-Ti systems, focusing on how Ti additions influence the thermodynamic stability of high-temperature HMs. Two compositional pathways were examined: one dominated by Sm/Ce-Fe/Co binary chemistry and the other influenced by (Sm/Ce)-(Fe/Co)-Ti ternary interactions. We employed ab initio calculations to investigate the finite-temperature stability of ordered, disordered, and metastable phases, thereby guiding experiments. Based on the computed energetics, we analyzed how Ti incorporation alters local bonding environments and stabilizes magnetically desirable motifs. Furthermore, we constructed an ab initio phase diagram to reveal the interplay between rare-earth metals and transition metals across a broad temperature range. We have revealed that Ti addition promotes the formation of a more robust Sm-rich phase by strengthening the local Sm-Fe-Ti matrix. This stabilization enhances alloy coercivity and provides insights into the thermodynamic and chemical factors driving phase evolution, enabling the design of better permanent HMs.

FM 9.5 Tue 15:15 BEY/0138

**Molecular orbital degeneracy lifting in NbSeI** — •Keita Kojima[1], Hayato Takano[1], Youichi Yamakawa[2], Shunsuke Kitou[3], Ryutaro Okuma[1], and Yoshihiko Okamoto[1] — [1]Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan

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The breathing pyrochlore lattice, composed of alternating small and large tetrahedra, hosts molecular orbitals within the smaller tetrahedra that strongly influences its physical properties. Such molecular-orbital and frustration-driven effects have led to diverse electronic states in related compounds. We investigated NbSeI, a MoSBr-type material with a particularly large breathing distortion whose physical properties remain unexplored despite previous synthesis reports. We synthesized single crystals and conducted x-ray diffraction, physical property measurements, and first-principles calculations. While the calculations predict metallic flat bands originating from Nb 4d orbitals, magnetic and transport measurements reveal a nonmagnetic insulating state below 300 K. NbSeI also undergoes a structural transition at Ts = 106 K. Our structural studies demonstrate local atomic displacements above Ts and a trimer-like molecular transformation below Ts. Our results show that the combination of strong breathing distortion and flat-band*derived electronic structure stabilizes molecular-orbital degrees of freedom, advancing orbital physics beyond single-ion descriptions toward cluster-based electronic phenomena.