MM 15: Phase Transformations II

Time: Monday 16:45–18:00 Location: C 230

MM 15.1 Mon 16:45 C 230

Quantum hydrogen bond symmetrization in water ice and sulfur hydride — •Marco Cherubini and Michele Casula — Institut de Minéralogie, de Physique de Matériaux et de Cosmochimie, CNRS, Paris, France

Hydrogen bond symmetrization, influenced by the quantum nature of protons, is expected in various compounds. Nuclear quantum fluctuations diminish the boundary between symmetric and asymmetric phases by several gigapascals. Here, we investigate water ice and sulfur hydride, compounds exhibiting hydrogen bond symmetrization and sharing deep analogies. We use path integral molecular dynamics and the self-consistent harmonic approximation in combination with Quantum Monte Carlo, ab initio calculations, and machine learning potentials to solve the nuclear and electronic problems. In water ice, hydrogen bond symmetrization is a long-debated issue because of the lack of univocal experimental signatures. We describe, for the first time, the strong temperature dependence of the critical pressure in the classical regime, showing that quantum effects are so strong as to completely cover the thermal fluctuations, reducing the phase boundary by over 50 GPa. Importantly, we prove that proton disorder minimally influences quantum symmetrization. Sulfur hydride has been widely studied for its superconductivity, with its maximum critical temperature (200 K) previously believed to be associated with hydrogen bond symmetrization. Indeed, we prove that it is related to the transition from the symmetric phase to a phase characterized by disordered local moments, and that the asymmetric phase is reached at much lower pressures.

MM 15.2 Mon 17:00 C 230

Unusual spectral features in BaZrO3 — •Petter Rosander, Erik Fransson, Nicklas Österbacka, Paul Erhart, and Göran Wahnström — Chalmers university of technology, Gothenburg, Sweden

Barium zirconate $BaZrO_3$ is one of few perovskites that retains an average cubic structure down to 0 K at ambient pressure. Despite this, it shows unusually sharp features in the Raman spectrum, which are supposed to be absent in a cubic system. In addition, a sharp reflection in electron diffraction appears at the R-point of the crystal at low temperatures. It has been suggested that these features are due to that the local structure of $BaZrO_3$ may form nanodomains or a glass-like phase at low temperatures.

Here, the static structure factor of $BaZrO_3$ is calculated as a function of temperature and pressure via molecular dynamics simulations using a machine-learned potential with near density functional theory (DFT) accuracy. A dielectric tensor model is also trained with near DFT accuracy to calculate the Raman spectrum as a function of pressure using molecular dynamics simulations.

We show that the sharp features in the Raman spectrum is due to higher order scattering and that the sharp reflection observed in electron diffraction is diffuse superlattice reflections that stems from the onset of a phase transition that never occurs.

MM 15.3 Mon 17:15 C 230

Electronic and atomic structure analysis of $Fe_4(P_2O_7)_3$ crystal — •Svitlana Pastukh[1,2], Pawel Jochym[2], Dominik Legut[1], and Przemysław Piekarz[2] — [1]IT4Innovations, VSB-Technical University of Ostrava, 708 00 Ostrava, Czech Republic — [2]Institute of Nuclear Physics, Polish Academy of Sciences, PL-31342 Kraków, Poland

This research delves into a comprehensive investigation of the electronic, magnetic, and structural characteristics of the $Fe_4(P_2O_7)_3$ crystal through first principles calculations utilizing DFT. Employing the GGA within VASP, our study focused on elucidating the properties of the crystal lattice, which adopts a monoclinic structure under space group $P2_1|n$. The optimized lattice parameters were determined as a=7.409 Å, b=21.425 Å, c=9.529 Å, with a unit cell containing four molecules (Z=4). It was shown that by taking into account van der Waals corrections, we aimed to improve the treatment of dispersion interactions and enhance the accuracy of the crystal structure optimization. Our examination encompasses the electronic and lattice attributes, considering four distinct magnetic configurations. The investigation revealed the AFM-1 configuration to possess the lowest total energy, exhibiting magnetic moments of 4.598 μ_B on Fe atoms. Additionally, for the relaxed crystal structure, we conducted analyses of the phonon dispersion relations and phonon density of states through the temperature-dependent effective potential method. These comprehensive findings contribute significantly to enhancing our understanding of the $Fe_4(P_2O_7)_3$ crystal, shedding light on its potential applications across various scientific domains.

MM 15.4 Mon 17:30 C 230

Phase transitions in 2D halide perovskites using machine learned potentials — •Erik Fransson, Julia Wiktor, and Paul Erhart — Chalmers University of Technology, Sweden

Two dimensional hybrid halide perovskite is a class of materials with interesting and useful optoelectronic properties for many applications areas, such as solar cells. These structure consists of one or a few layers of the perovskite phase connected via organic spacer molecules, and they can for example exhibit increased stability compared to their 3D counterparts.

Here, we make use of machine learning potentials, with near DFT accuracy, and large-scale molecular dynamics simulations in order to investigate thermodynamic properties and stability of these complex structures for the prototypical spacer molecule phenethylammonium (PEA). The phase transitions can directly be observed via structural parameters such as octahedral tilt angles and bond-lengths. Interestingly, we find that the phase transitions in the single perovskite layer structure appears at a significantly higher temperature and with different character compared to the 3D perovskite phase. We analyze the phase transitions temperature and character with varying number of perovskite layers in order to understand how the phase transition property changes as a function of dimensionality in the system. We observe surface effects for the thicker perovskite systems, such as the surface layers exhibiting stronger octahedral tilt and undergo the phase transitions at higher temperatures (about 50K) compared to the bulk-layers.

MM 15.5 Mon 17:45 C 230

MT6Z6 kagome candidates with flat bands, magnetism, phonon instability, and charge density waves — •Xiaolong Feng[1], Yi Jiang[2], Haoyu Hu[2], Dumitru Călugăru[3], Maia Garcia Vergniory[1,2], Claudia Felser[1], Santi Blanco-Canosa[2], and Bogdan Andrei Bernevig[2,3,4] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Donostia International Physics Center(DIPC), Paseo Manuel de Lardizábal. 20018, San Sebastián, Spain — [3]Department of Physics, Princeton University, Princeton, NJ 08544, USA — [4]IKERBASQUE, Basque Foundation for Science, 48013 Bilbao, Spain

Kagome materials manifest rich physical properties due to the emergence of abundant electronic phases at different fillings. Here, we carry out a high-throughput first-principles study of the MT6Z6 kagome materials, regarding their electronic flat bands and lattice instability. The diverse MT6Z6 kagome candidates reveal the remarkable tunability of kagome flat bands from unfilled and fully filled states. Mn/Fe-166 compounds exhibit partially filled flat bands with a pronounced sharp DOS peak near the Fermi level, suggesting the presence of magnetic orderings, which split the sharp DOS peak and stabilize the phonon. When the flat bands are located away from the Fermi level, the instabilities can be classified into three types, regarding their vibration modes. Type-I instabilities involve the in-plane distortion of kagome nets, while type-II and type-III present out-of-plane distortion of trigonal M and Z atoms. Our prediction suggests a vast kagome family for the exploration of rich properties induced by the flat bands.