MM 65: Functional Materials (Actuators, filters, sensors, shape memory)

Time: Thursday 17:30–19:00 Location: H 0106

MM 65.1 Thu 17:30 H 0106

Thermosalient ('jumping') crystals — •Ivor Lončarić[1], Jasminka Popović[1], Vito Despoja[2], and Željko Skoko[2] — [1]Ruđer Bošković Institute, Bijenička 54, HR-10000 Zagreb, Croatia — [2]Department of Physics, Faculty of Science, University of Zagreb, Bijenička 32, HR-10000 Zagreb, Croatia

Thermosalient materials when heated or cooled are characterized by a fast and energetic phase transition in which crystals experience macroscopic change in dimensions and jump to distances much larger than their own dimension. Since the first systematic study [1], there has been a rising intrest for these interesting, and potentially useful, acutating materials. As a one example, N-2-propylidene-4-hydroxybenzohydrazide shows irreversible thermosalient phase transition from Form I to Form II and reversible thermosalient phase transition from Form II to Form III. We combine experiments and first-principles electronic structure calculations to elucidate this interesting and technologically useful phenomenon[2].

[1] Skoko et al., J. Am. Chem. Soc. 132, 14191 (2010)

[2] Lončarić et al., Cryst. Growth Des. 17(8), 4445-4453 (2017)

MM 65.2 Thu 17:45 H 0106

Analysis of different methods for methylammonium lead iodide perovskite deposition into nanoporous anodic-aluminum oxide membranes — •Mirko Gabski, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

Organometal-trihalide perovskites are organo-metal salts which have gained popularity as a light harvesting material in thin film solar cells in recent years due its favorable properties (e.g. cheap and simple processing, high absorption coefficient, direct band gap, high charge carrier mobility) and led to solar cells with efficiencies up to $\sim$20 %. Anodic-aluminum oxide (AAO) provides a highly ordered nanoporous template consisting of hexagonally arranged pores with tunable pore diameters ranging from $\sim$10 to $\sim$200 nm and a thickness between $\sim$10 nm and 100 μm which is easily synthesized using a simple anodization procedure and is thus excellently suited for the synthesis of quasi-one-dimensional nanostructures. By choosing a suitable deposition method the AAO template can be used to fabricate an array of quasi-one-dimensional perovskite nano-rods in parallel circuit where the direction of charge carrier flow is guided by the confinement imposed by the surrounding AAO. In this work, different deposition methods (e.g. drop-coating, dip-coating, spin-coating and co-evaporation) are investigated for their applicability for perovskite deposition into AAO membranes with varying thicknesses and pore diameters since changing aspect ratios impose different constraints on the choice of the most suitable deposition method.

MM 65.3 Thu 18:00 H 0106

Role of Hydrogen Bonds in Organic Ferroelectrics using Neutron Scattering and First principles Simulations — •Sanghamitra Mukhopadhyay — ISIS Facility, Rutherford Appleton Laboratory-STFC, Harwell Science and Innovation Campus, Oxfordshire OX11 0QX, UK

Hydrogen bonded organic ferroelectrics are important functional materials for potential technological applications in flexible electronics. Role of hydrogen bonds is important in this class of materials for designing new functionalities. Microscopic knowledge of structure and dynamics of those hydrogen bonds are thus crucial. In this work I will present structure and dynamics of few organic ferroelectrics using neutron diffraction, spectroscopy and first principles simulations.

Neutron scattering experiments are done on IRIS and OSIRIS spectrometers at ISIS to understand the structures and hydrogen bond motifs in these ferroelectrics. inelastic and quasielstic neutron scattering spectroscopies are employed to investigate the pico-second dynamics in those materials.

State-of-the-art calculations based on plane wave pseudo potential density functional theory to predict the structure. Inelastic neutron scattering spectrum are interpreted using first principles lattice dynamics and the quasielastic neutron spectrum are calculated by analysing the trajectory of the molecular dynamical simulations.

Correlating structure and dynamics of these functional materials, it is shown that the in-plane strains on hydrogen bonds are responsible for high ferroelectric polarisation of these organic solids.

MM 65.4 Thu 18:15 H 0106

In situ observations on dynamic reconfiguration of bilayer defects in van der Waals bonded Ge-Sb-Te based alloys — •Andriy Lotnyk[1], Ulrich Ross[1], Torben Dankwort[2], Isom Hilmi[1], Lorenz Kienle[2], and Bernd Rauschenbach[1,3] — [1]Leibniz Institute of Surface Engineering (IOM), Permoserstr. 15, 04318 Leipzig, Germany — [2]Institute for Materials Science, Faculty of Engineering, University of Kiel, Kaiserstr. 2, 24143 Kiel, Germany — [3]Felix Bloch Institute for Solid State Physics, Leipzig University, Linnéstr. 5, 04103 Leipzig, Germany

Ge-Sb-Te (GST) based phase change alloys are well-known materials from optical data storage applications and are emerging contenders for non-volatile data storage applications. In the present work, atomic structure and dynamics of layered defects frequently reported in van der Waals bonded GST based alloys and superlattices are investigated using aberration-corrected STEM. The defects are confined into two atomic layers of GeSb and Te and represent special type of stacking fault. In situ experiments showed that the bilayers can be easily reconfigured into such bilayer stacking faults with subsequent formation of a new van der Waals gap. Depending on the beam dose, the newly formed stacking fault can either reconfigure back to the initial state or move in later direction within the faulty stacking plane. The results of the present work shed insight into mechanism of structural reconfiguration of building blocks in van der Waals bonded GST compounds, also relevant for an understanding of switching mechanisms in iPCMs.

MM 65.5 Thu 18:30 H 0106

Stability of the Shape Memory Effect and Transformation Temperatures in Ti-Ta-X Alloys — •Alberto Ferrari, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, 44801 Bochum, Germany

Ti-Ta-based alloys exhibit a high-temperature shape memory effect (SME) due to a martensitic transformation between an orthorhombic phase (α'') and a body-centered cubic phase (β). The stability of the SME in binary Ti-Ta is compromised by the formation of detrimental phase (ω). It has been observed experimentally that alloying a third component to pure Ti-Ta hinders the formation of the ω phase. Both the stability of the SME and the transformation temperature depend strongly on the chemical composition; the underlying mechanism is, however, not fully understood. In this contribution, the stability and the transformation temperature are analyzed systematically as a function of composition of Ti-Ta-X by means of *ab-initio* calculations; in particular, it is examined how different elements and different concentrations affect the formation energy of the α'', β and ω phases. The trends in formation energies are found to be related to the electronic properties and the size of the alloying elements. Simpler models that describe the compositional dependence of the transformation temperature are derived from first principles data and allow us to gain chemical insight into the effect of alloying on the relative phase stability. Our model is exploited to guide the experimental design of new stable and high-temperature shape memory alloys.

MM 65.6 Thu 18:45 H 0106

Functionalized gold electrodes for sensing DNA mutations — Ganesh Sivaraman[1], Frank C. Maier[1], Rodrigo Amorim[2], Ralph H. Scheicher[3], and •Maria Fyta[1] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Universidade Federal Fluminense, Departamento de Física, Volta Redonda/RJ, Brazil — [3]Department of Physics and Astronomy, Materials Theory, Uppsala University, Sweden

Derivatives of small diamond-like nanostructures, the diamondoids, are used to functionalize fold electrodes. Within the gap of these functionalized electrodes, different DNA units are placed. These are native nucleotides, as well as modified nucleotides, such as mutations and epigenetic markers. Using quantum-mechanical calculations together with the non-equilibrium Green's functions formalism, we investigate the electronic transport properties across the functionalized electrodes for the cases of all nucleotides place in the electrode gap. Distinct electronic signals were found, which give rise to different coupling strengths across the electrode gap. These signals occur at distinct values of the gating voltage and can uniquely characterize the nucleotide in the metallic gap. Specifically, they can clearly distinguish between the native and the mutated nucleotides. Accordingly, diamondoid functionalized electrodes can be used as a sensing setup within nanopore materials.