FM 15: Nanoscale Probing of Functional Properties

chair: Jiali He (Norwegian University of Science and Technology, Norway)

Time: Wednesday 15:00–15:45 Location: BEY/0E40

FM 15.1 Wed 15:00 BEY/0E40

Nanoscale Phonon Dynamics Studied In-Situ by Laser Stimulated Vibrational Electron Energy-Gain Spectroscopy — •Mairi McCauley[1,2], Joel Martis[3], Ondrej Krivanek[3], Ben Plotkin-Swing[3], Tolga Wagner[1,2], Hüseyin Çelik[1,4], Grigory Kornilov[1], Katrina Coogan[1,2], Meng Zhao[1,2], Andreas Mittelberger[3], Matthias Meffert[5], Luca Piazza[5], Tracy Lovejoy[3], Guillaume Radtke[6], Christoph Koch[1,2], and Benedikt Haas[1,2] — [1]Department of Physics, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Center for the Science of Materials Berlin, Humboldt-Universität zu Berlin, Berlin, Germany — [3]Bruker AXS LLC, Kirkland, WA, USA — [4]Institute for Physics and Astronomy, Technische Universität Berlin, Berlin, Germany — [5]DECTRIS AG, Baden-Daettwil, Switzerland — [6]Sorbonne Université, CNRS UMR 7590, MNHN, IMPMC, Paris, France

Advances in instrumentation allow to directly probe phonon dispersions at the nanoscale using electron energy gain and loss spectroscopy (EEGS/EELS) within a scanning transmission electron microscope (STEM). By integrating a laser injection system, we enable the investigation of stimulated phonons at the spatial resolution determined by the electron beam. A synchronised laser-detector configuration enables nanosecond-scale time-resolved measurements. The thermal conductivity of amorphous carbon and silicon nitride was investigated by local time-resolved temperature measurements and is compared to numerical simulations. Ongoing work applies the system to study phonon transport through defects and interfaces at atomic resolution.

FM 15.2 Wed 15:15 BEY/0E40

Photoluminescence Spectroscopy of Platinum (II) and Palladium (II) Dimers in Organic Molecular Single Crystals Under Pressure — Paul Steeger[1], Tobias Theiss[2], Dominik Schwab[3], Ivan Maisuls[2], •Vedhanth Senthiappan Vellaiappan Uthayasurian[1], Robert Schmidt[1], Ilya Kupenko[4], Carmen Sanchez Valle[4], Steffen Michaelis de Vasconcellos[1], Nikos L. Doltsinis[3], Cristian A. Strassert[2], and Rudolf Bratschitsch[1] — [1]Institute of Physics, University of Münster — [2]Institut für Anorganische und Analytische Chemie, University of Münster — [3]Institute of Solid State Theory, University of Münster — [4]Institute of Mineralogy, University of Münster

Cyclometalated transition-metal complexes are promising for applications ranging from bioimaging to light-emitting diodes. We investigate two tailored biscyclometalated Pd(II) and Pt(II) complexes, which feature ligands that promote head-to-tail dimer formation to enable interactions between their metal centers [1]. We prepare molecular single crystals and apply hydrostatic pressure with a diamond anvil cell in the GPa range [2]. The photoluminescence shows a prominent redshift under pressure. Density functional theory calculations link this effect to a reduced metal-metal distance. Importantly, the observed mechanochromism is reversible, which holds the promise for pressure sensing and optical storage applications. References: [1] T. Theiss et al., J. Am. Chem. Soc. 145, 3937 (2023), [2] P. Steeger et al., Nano Lett. 25, 2628 (2025)

FM 15.3 Wed 15:30 BEY/0E40

A novel Approach to parametrize a ferroelectric Phase-Field Model from atomistic Simulation Data — •Frank Wendler[1], Dilshod Durdiev[2], Xuejian Wang[1], Hikaru Azuma[3], Takahiro Tsuzuki[3], Tomohiro Ogawa[3], Ryo Kobayashi[3], Masayuki Uraganase[4], Shuji Ogata[3], and Michael Zaiser[1] — [1]Institute of Materials Simulation, FAU Erlangen-Nürnberg, Dr.-Mack-Str. 77, 90762 Fürth, Germany — [2]Division Mechanics of Functional Materials, TU Darmstadt, Germany — [3]Physical Science and Engineering Department, Nagoya Institute of Technology, Japan — [4]RIKEN Center for Biosystems Dynamics Research, Japan

Based on molecular dynamics simulations using a core-shell potential for polarization switching in ferroelectric BaTiO3 (BTO) with and without vacancy defects, a parametrization framework for phase-field simulations is established. Crucial material properties such as elastic and piezoelectric tensor components, kinetic coefficients, as well as domain wall characteristics are extracted from the MD results to adjust the anisotropic gradient energy. The 6th order Landau polynomial coefficients are derived from statistical analysis of polarization switching data, including the activation parameters for BTO that govern domain nucleation. The proposed energy landscape favours polarization switching in two subsequent 90° steps over 180° switching, which was observed experimentally and in recent MD simulations. The method is important for phase-field simulations of domain nucleation and domain wall motion in presence of point defects carrying mono- or dipolar electric fields as well as elastic strain fields.