MM 7: Microstructures and Phase Transformations: Oxides & Perovskites

Time: Monday 15:45–17:00 Location: H45

MM 7.1 Mon 15:45 H45

Evolution of a particle in twisted bilayer optical potentials — •Ganesh C. Paul[1], Patrik Recher[1,2], and Luis Santos[3] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, 38106 Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, 38106 Braunschweig, Germany — [3]Institut für Theoretische Physik, Leibniz Universität Hannover, Germany

Very recently few theoretical proposals have been put forward to simulate twisted bilayers using cold atoms in state-dependent optical lattices, which can be used as an alternative platform to investigate twisted bilayers in solid-state experiments. We study the band structure of both square and hexagonal geometries in an optical lattice set-up, where the band structure can be tuned to be almost flat by proper implementation of interlayer Gaussian-type coupling. We examine the evolution of a particle in the twisted bilayer square-like potential, and find that the particle follows specific paths forming channels when the interlayer hopping is much stronger than the intralayer hopping strength. Due to the flexibility of controlling the inter- and intralayer coupling in optical lattices, our proposals should be easy to be realised in a cold atom set-up.

MM 7.2 Mon 16:00 H45

Phase transitions and phonon renormalization in $CsPbBr_3$ via a machine learning interatomic potential — •Erik Fransson[1], Fredrik Eriksson[1], Petter Rosander[1], Terumasa Tadano[2], and Paul Erhart[1] — [1]Chalmers University of Technology, Gothenburg, Sweden — [2]National Institute for Materials Science, Tsukuba, Japan

Here, we present a study on phase-transition and phonon renormalization in the metal halide perovskite $CsPbBr_3$ using a machine learning (ML) interatomic potential. The ML potential is a neuroevolution-potential constructed using the GPUMD software and is trained on atomic forces, energies and stresses obtained from DFT calculations. We find that the ML potential captures the correct phase-transition from the orthorhombic phase to tetragonal phase and from tetragonal to cubic phase. The phase transition temperatures obtained are slightly underestimated compared to experimental studies, but in good qualitative agreement. These phase-transitions are connected to the so called tilt-modes at the R and M point in the brillouin zone, which corresponds to tilting of the $PbBr_6$ octahedra. The dynamics of these modes are studied with MD simulations and mode projections, and we find that they have are strongly anaharmonic and over-damped character. Furthermore, we investigate and benchmark how different self-consistent phonon methods work for these strongly anharmonic modes.

MM 7.3 Mon 16:15 H45

A particular EFG temperature dependence for 181-Ta(TiO2): An electron-gamma TDPAC study — •Ian Chang Jie Yap[1], Juliana Schell[2,3], Thien Thanh Dang[3], Cornelia Noll[4], Reinhard Beck[4], Ulli Köster[5], Ronaldo Mansano[6], Peter Blöchl[1,7], and Hans Christian Hofsäss[1] — [1]Georg-August Universität Göttingen — [2]European Organization for Nuclear Research (CERN) — [3]Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen — [4]Helmholtz-Institut für Strahlen- und Kernphysik, University of Bonn — [5]Institut Laue-Langevin — [6]Escola Politécnica, Universidade de São Paulo — [7]Technische Universität Clausthal, Institute of Theoretical Physics

In this work, we report on the hyperfine parameters of the implanted 181Ta probe in the rutile structure of the single crystal TiO2 using the e - γ time differential perturbed angular correlation (e - γ TDPAC) technique. The experiments were performed under vacuum within the temperature range of 50 K - 427 K. The hyperfine parameters that are obtained from the e - γ TDPAC spectroscopy agrees with that of the γ - γ TDPAC spectroscopy at room temperature, apart from a calibration factor, both from our experiments and literature. Surprisingly, we have detected a parabolic increase of Vzz with a concave curvature at the low-temperature regime (50 K - 427 K), as opposed to the linear increase at the high-temperature regime (600 K - 1200 K) as found in the literature. Hence, we are performing DFT calculations on Ta-doped TiO2 over a broad temperature range to obtain deeper insights.

MM 7.4 Mon 16:30 H45

Hidden charge order in square-lattice $Sr_3Fe_2O_7$ — •Darren C. Peets[1,2,3], Jung-Hwa Kim[1], Manfred Reehuis[4], Peter Adler[5], Andrey Maljuk[1,6], Tobias Ritschel[2], Morgan C. Allison[2], Jochen Geck[2,7], Jose R. L. Mardegan[8], Pablo J. Bereciartua Perez[8], Sonia Francoual[8], Andrew C. Walters[1,9], Thomas Keller[1,10], Paula M. Abdala[11], Philip Pattison[11,12], Pinder Dosanjh[13], and Bernhard Keimer[1] — [1]MPI-FKF, 70569 Stuttgart — [2]IFMP, TU Dresden, 01069 Dresden — [3]NIMTE CAS, Ningbo, 315201 China — [4]HZB, 14109 Berlin — [5]MPI-CPfS, 01187 Dresden — [6]IFW, 01171 Dresden — [7]ct.qmat, TU Dresden, 01062 Dresden — [8]DESY, Hamburg 22603 — [9]Diamond, Didcot OX11 0DE, UK — [10]MPI Outstation at MLZ, 85748 Garching — [11]SNBL at ESRF, 38042 Grenoble, France — [12]EPFL, BSP-Dorigny, CH-1015 Lausanne, Switzerland — [13]UBC, Vancouver, V6T 1Z1 Canada

Since the discovery of charge disproportionation in $Sr_3Fe_2O_7$ by Mössbauer spectroscopy >50 years ago, the spatial ordering pattern of the disproportionated charges has stayed "hidden" to conventional diffraction, despite numerous x-ray and neutron studies. Our neutron Larmor diffraction and Fe K-edge resonant x-ray scattering demonstrate checkerboard charge order in the FeO_2 planes that vanishes at a sharp second-order phase transition at 332 K. Stacking disorder of the checkerboard pattern due to frustrated interlayer interactions broadens their superstructure reflections, greatly reducing their amplitude, explaining the difficulty to detect them. We discuss implications of these findings for research on "hidden order" in other materials.

MM 7.5 Mon 16:45 H45

Band structure effects of a current-induced Mott-insulator to metal transition in Ca_2RuO_4 — •D. Curcio[1], C. E. Sanders[2], A. Chikina[1], M. Bianchi[1], H. E. Lund[1], V. Granata[3], M. Cannavacciuolo[3], P. Dudin[4], J. Avila[4], C. Polley[5], B. Thiagarajan[5], A. Vecchione[6], and P. Hofmann[1] — [1]Department of Physics and Astronomy, Aarhus University, Denmark — [2]STFC Central Laser Facility, Harwell Campus, United Kingdom — [3]Dipartimento di Fisica *E.R. Caianiello*, Università degli Studi di Salerno, Italy — [4]Synchrotron SOLEIL, Gif-sur-Yvette, France — [5]MAX IV Laboratory, Lund University, Lund, Sweden — [6]CNR-SPIN, c/o Università degli Studi di Salerno, Italy

The Mott insulator Ca_2RuO_4 can be turned into a metal by the application of a weak electric field and a corresponding transport current. This transition affects the optical and magnetic properties of the material. However, because of the electric field's presence and the field-induced energy broadening, it is challenging to determine the electronic structure in the metallic state by angle-resolved photoemission spectroscopy (ARPES). Making use of the recently introduced approach to enable ARPES measurements of current-carrying devices by using a nano-scale light spot [1], we are able to measure ARPES data that tracks the current-induced phase transition in Ca_2RuO_4 simultaneously with the electrical transport, revealing the spectral function of the current-induced state along with a potential map of the sample's surface.

[1] D. Curcio *et al.* Phys. Rev. Lett. 125, 236403 (2020).