O 22: Poster Session II: New methods II

Time: Monday 13:30–15:30 Location: P

O 22.1 Mon 13:30 P

Enabling size convergence for surface calculations of materials exhibiting spontaneous polarization — •Su-Hyun Yoo[1], Mira Todorova[1], Liverios Lymperakis[1], Chris Van de Walle[2], and Jörg Neugebauer[1] — [1]Department of Computational Materials Design, Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Materials Department, UCSB, USA

The most common approach to describe surfaces in density-functional theory is the repeated slab geometry based on periodic boundary conditions. A common strategy to avoid artificial charge transfer from one side of the slab to the other when modelling semiconductor surfaces is to passivate partially filled surface dangling bonds at the backside of the slab. Using the example of wurtzite (0001) surfaces we demonstrate that conventionally used passivation schemes (e.g. pseudo H or surface reconstructions) break down for materials exhibiting spontaneous polarization. We have therefore developed a generalized passivation method that accounts for the effect of spontaneous polarization and correctly describes the asymptotic bulk limit for pyroelectric materials. It is robust and ensures quick convergence of total energies and electronic structure with respect to system size. The performance of our approach will be demonstrated using the example of wurtzite ZnO polar [1] and wurtzite GaN semi-polar surfaces [2].

[1] S. Yoo, M. Todorova, D. Wickramaratne, L. Weston, C. Van de Walle, and J. Neugebauer, NPJ Computational Materials (submitted).

[2] S. Yoo, L. Lymperakis, and J. Neugebauer (in preparation).

O 22.2 Mon 13:30 P

WannierBerri code - a fast python code for Wannier interpolation. — •Stepan Tsirkin[1], Xiaoxiong Liu[1], Minsu Ghim[2], Patrick Lenggenhager[2,3,6], Iñigo Robredo[4], Miguel Ángel Jiménez Herrera[5], Ji Hoon Ryoo[2], Jae-Mo Lihm[2], Cheol-Hwan Park[2], and Ivo Souza[5] — [1]University of Zurich — [2]Seoul National University — [3]ETH Zurich — [4]Donostia International Physics Center, Spain — [5]CFM, Universidad del País Vasco, Spain — [6]Paul Scherrer Institute, Villigen PSI, Switzerland

We present WannierBerri (WB) [1] - a new Python code for Wannier interpolation, which is close in spirit to the postprocessing module of the well-known Wannier90 code [2] (postw90.x), but improves over it by implementing a number of methodological advances [3], which boost the speed of computations by orders of magnitude, enabling to study more complex materials with higher accuracy without demanding enormous computational resources. A plethora of quantities are implemented, such as anomalous Hall conductivity, orbital magnetization, Berry curvature dipole, and spin Hall conductivity, among many others. WB is also capable of evaluating analytical covariant derivatives of the Berry curvature and orbital moment, which allows to study different magnetotransport phenomena, and also to implement Fermi-sea formulations of Berry dipole.

[1] http://wannier-berri.org

[2] http://wannier.org

[3] https://arxiv.org/abs/2008.07992

O 22.3 Mon 13:30 P

Frequency and momentum-resolved detection of non-thermal gigahertz phonons with Fano coupling to charge carriers — •Thomas Vasileiadis[1], Heng Zhang[2], Hai Wang[2], Mischa Bonn[2], George Fytas[2], and Bartlomiej Graczykowski[1] — [1]Faculty of Physics, Adam Mickiewicz University, Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland. — [2]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany.

Spontaneous micro-Brillouin light scattering (μ-BLS) can probe gigahertz acoustic phonons in nano-confined materials with momentum and spatial resolution. However, the downsizing of the scattering volume implies weak BLS signals, sample overheating, and damage [1]. In this work, we present pumped-BLS [2], an all-optical technique that generates non-thermal acoustic phonons with ultrashort laser pulses and probes them with frequency- and momentum-resolution. Using pumped-BLS we show: (i) a hundred-fold enhancement of BLS spectra, compared to equilibrium, of 260 nm thick Si membranes due to photoexcited non-thermal gigahertz phonons, (ii) Stokes / anti-Stokes asymmetry due to asymmetric non-thermal phonon propagation and (iii) strongly asymmetric Fano resonances due to coupling between the electron-hole pairs and the phonons. This project is funded from NCN (UMO-2018/31/D/ST3/03882), ERC (grant no. 694977) and FNP (POIR.04.04.00-00-5D1B/18). TV acknowledges funding from the European Union's Horizon 2020 research and innovation programme. [1] M. Sledzinska, et al. Adv. Funct. Mater. 30 (8), 2020. [2] Th. Vasileiadis et al. Science Advances 6 (51), eabd4540, 2020.

O 22.4 Mon 13:30 P

Bound in the continuum modes in indirectly-patterned hyperbolic media — •Hanan Herzig Sheinfux[1], Lorenzo Orsini[1], Minwoo Jung[2], Iacopo Torre[1], Matteo Ceccanti[1], Eli Janzen[3], James Edgar[3], Gennady Shvets[2], and Frank H Koppens[1] — [1]ICFO, Spain — [2]Cornell university, USA — [3]Kansas state university, USA

Conventional optical cavities support one or more modes, which are unable to leak out of the cavity. Bound state in continuum (BIC) cavities are an unconventional alternative, where there are available channels for the mode to leak through, but it remains confined due to destructive interferences. BICs are a general wave phenomenon. It is interesting to consider BICs in the context of hyperbolic media (HyM), as a way to produce cavties with extremely small mode volume and enhanced light matter interaction. However a hyperbolic BIC cavity presents a fundamental challenge, since the cavity's HyM cladding supports an infinite number of modes which would need to interfere. Here, we introduce hyperbolic BICs (hBICs) and construct the first BIC-based nanocavities. These hBICs are formed through a novel multimodal reflection spatial mechanism, to do with the vanishing spatial overlap between ray-like excitations in a HyM and all leakage channels. Using near-field microscopy, we directly observe this asymmetrically enhanced reflection and demonstrate mid-IR nanocavities with volumes down as small as 15x15x3nm and quality factors reaching above 100, a dramatic improvement in several metrics of confinement.

O 22.5 Mon 13:30 P

Elucidation of Disordered Mesopore Constructs: A Kernel-Based Approach — •Henry R. N. B. Enninful, Dirk Enke, and Rustem Valiullin — Leipzig University

Detailed characterisation of the structure of mesoporous solids presents key insights into the accurate design of various industrial applications such as catalysis, molecular separations and adsorption, among others. Routine characterisation tools, such as gas sorption, typically utilise the general adsorption isotherm (GAI) equation derived for ordered pore systems. For disordered porous solids, the complex morphology with its resulting cooperativity effects in thermodynamic phase transitions renders characterisation more complex than what the GAI supports.

Herein, we present a kernel-based approach with the serially connected pore model (SCPM); an extension of the GAI which incorporates cooperativity effects in phase transitions arising from pore complexity. Modelled as a statistical linear chain of pores, the SCPM is validated with data from solid-liquid phase transitions of water in synthesized porous silica material of similar pore construct, MCM-41. To show its robustness, we employ the SCPM to reveal disorder in SBA-15 mesoporous solid.

O 22.6 Mon 13:30 P

Single-Hemisphere Photoelectron Momentum Microscope with Time-of-Flight Recording — •Gerd Schönhense, Sergey Babenkov, Dmitry Vasilyev, Hans-Joachim Elmers, and Katerina Medjanik — Johannes Gutenberg-Universität, Institut für Physik, 55128 Mainz, Germany

Photoelectron momentum microscopy is an emerging powerful method for angle-resolved photoelectron spectroscopy (ARPES). These instruments record k_x - k_y images, typically exceeding a full Brillouin zone. As energy filters double-hemispherical [1] or time-of-flight (ToF) [2] devices are in use. Here we present a new approach for momentum mapping of the full half-space, based on a large single hemispherical analyzer [3]. Excitation by an unfocused He lamp yielded an energy resolution of 7.7 meV. The method circumvents the preconditions of previous theoretical work on the resolution limitation due to the alpha-square term and the transit-time spread (detrimental for time-resolved

experiments). Data recording in the Fourier plane allows for large range of entrance angles in the analyzer (up to ±7°, opposed to typically ±2° in conventional analyzers). A dispersive-plus-ToF hybrid mode with ToF analyzer behind the exit slit yields a gain up to N^2 in recording efficiency (N number of resolved time slices). A key application will be ARPES at sources with high pulse rates like synchrotrons with 500 MHz time structure; the prototype will be installed at Diamond, UK. [1] C. Tusche et al., Ultramicrosc. **159**, 520 (2015); [2] K. Medjanik et al., Nature Mat. **16**, 615 (2017); [3] G. Schönhense et al., Rev. Sci. Instrum. **91**, 123110 (2020).