O 48: Poster Surface Dynamics

Time: Tuesday 18:00–20:00 Location: P2

O 48.1 Tue 18:00 P2

Atomistic modeling of ultrafast laser induced structural changes in Bismuth — •Sahar Bakhshi Sangari, Jimiben Patel, Bernd Bauerhenne, and Martin Garcia — Institute of Physics, University of Kassel, Kassel, Germany

We present a temperature-dependent interatomic potential for laser-excited bismuth, $\Phi_{Bi}(Te)$, developed using a database of temperature-dependent density functional theory (DFT) calculations. Bismuth is a widely studied material in experiments, yet theoretical studies exploring its atomic dynamics following femtosecond laser excitation remain scarce. Our work compares the physical properties predicted by $\Phi_{Bi}(Te)$ with those obtained from ab initio simulations, demonstrating its reliability. We use $\Phi_{Bi}(Te)$ to describe, in the framework of a generalized two-temperature-model molecular dynamics (TTM-MD) method, laser induced thermal and nonthermal ultrafast structural changes in Bi. We compute the time evolution of selected Bragg peaks and directly compare them with experimental observations. This approach enables efficient and accurate modeling of complex material behaviors, providing a valuable alternative to computationally intensive temperature-dependent DFT simulations.

O 48.2 Tue 18:00 P2

Design and Characterization of Optical Cavities for Light-Induced Phase Transitions in Indium-Based Peierls Insulators — •Florian Spickmann[1,2], Sierra Randall Heinrich[1,2], Sebastian Zafra Koch[1,2], Murat Sivis[1,2], Hannes Boeckmann-Clemens[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany

The integration of quantum materials into optical cavities enables active control of their properties through enhanced light-matter interactions. Low-dimensional materials, such as Peierls insulators, are particularly sensitive to external stimuli, making them ideal candidates for such studies [1]. This work focuses on designing and fabricating optical resonators on (111) silicon membranes, including slab waveguides, ridge waveguides, and ring resonators. The structures are created using focused ion beam (FIB) milling and electron beam lithography (e-beam), with light coupling achieved via integrated gratings. Characterization of the resonators is performed using Fabry-Pérot interferometry. Future studies will employ ultrafast low-energy electron diffraction (ULEED) to visualize light-driven phase changes in indium wires localized on these optical resonators, representing a promising model system for cavity-controlled light-matter interaction in condensed matter.

[1] Böckmann, Hannes, et al., Structural Dynamics 9.4 (2022)

O 48.3 Tue 18:00 P2

Ultrafast LEED Study of Bismuth Thin Films on Silicon (001) — •Nandana V Uday[1], Felix Kurtz[1], Jonas Fortmann[3], Alp Akbiyik[1], Michael Horn-von-Hoegen[3,4], and Claus Ropers[1,2] — [1])Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, 37077 Göttingen, Germany — [2]4th Physical Institute ,Solids and Nanostructures, University of Göttingen, 37077 Göttingen, Germany — [3]University of Duisburg-Essen, 47057 Duisburg, Germany — [4]Center for Nanointegration (CENIDE), 47057 Duisburg, Germany

The interface between two materials in a heterostructure serves as a barrier to the diffusion of thermal energy, thereby hindering heat flow across the boundary. On the nanoscale, heat transport may further be modified. Recently, it was shown that the thermal transport from Bi film into a Si substrate is reduced for films thinner than the phonon mean free path, due to phonon trapping by total internal reflection [1]. To study the non-equilibrium phonon dynamics in this process, ultrafast low-energy electron diffraction (ULEED) is suitable and direct means providing ultrafast temporal and high momentum resolutions. By analyzing the momentum-resolved map of a transient inelastic scattering background [2], we aim to identify phonon trapping, depopulation, and thermalization. As a first step, we monitor the heat transfer by phonons through the thin film-substrate interface, extracting cooling times from the transient lattice temperature of the bismuth film.

O 48.4 Tue 18:00 P2

Predicting and modelling incommensurate charge density waves in 1H-TaSe$_2$ via downfolding approach — •Clara Pfister[1,2], Laura Pätzold[1], and Tim O. Wehling[1,2] — [1]I. Institute of Theoretical Physics, U Hamburg — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg

Studying the emergence and thermodynamic behaviour of symmetry-broken phases such as charge density waves (CDWs) in solids is of great interest to deepen our understanding of collective phenomena and interactions between electrons and the crystal lattice. Incommensurate CDWs (ICCDWs) are especially intriguing because a realistic and efficient computational method to predict them has not been developed yet. To model ICCDW phases in the exemplary transition metal dichalcogenide material 1H-TaSe$_2$, we employed a downfolding approach that reduces the electronic degrees of freedom by retaining only the low-energy subspace relevant to CDW formation. This method achieves a computational speed-up of approximately five orders of magnitude compared to purely ab initio calculations [1], making it possible to simulate sufficiently large supercells efficiently. Our approach allows for modelling the ICCDW with reasonable accuracy, with the predicted temperature range for its occurrence agreeing well with experimental results of the ICCDW in undoped 2H-TaSe2 [2]. This suggests that our approach is applicable for the description of other materials exhibiting ICCDWs.

[1] A. Schobert et al., *SciPost Phys.* **16**, 046 (2024)

[2] X. Shen et al., *Nat. Commun.* **14**, 7282 (2023)