SFB1242

SFB 1242 Nichtgleichgewichtsdynamik kondensierter Materie in der Zeitdomäne

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Nonequilibrium dynamics of crystal lattices

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The coupling between electronic and vibrational degrees of freedom influences profoundly the ultrafast dynamics of electrons [1] and phonons [2]. Ab-initio calculations of the electron-phonon interaction (EPI), however, are typically confined to the study of systems at equilibrium and are thus unsuitable for the description of ultrafast phenomena. To circumvent these limitations, we develop an approach to study the coupled electron-phonon dynamics by combining semi-classical theories of carrier dynamics (as, e.g., non-thermal lattice models and the Boltzmann equation) with predictive many-body calculations of the EPI. We apply this formalism to explore the characteristic fingerprints of the EPI in systems driven out of equilibrium by the interaction with ultra-short light pulses [3].

For the prototypical two-dimensional semiconductor MoS_2, our calculations reveal a non-equilibrium lattice dynamics characterized by a striking anisotropy in reciprocal space, with phonon being emitted exclusively in the vicinity of high-symmetry points owing to phase-space constraints. This behaviour underpins the emergence of a non-thermal vibrational state of the lattice [4], whereby a highly anisotropic population of different phonons in the Brillouin zone is established and persists for up to 10 ps. For the layered semiconductor black phosphorus, these findings are corroborated by femtosecond electron diffuse scattering (FEDS) experiments [3].

The control of non-thermal vibrational states may provide unexplored opportunities to selectively enhance the phonon population and, thereby, transiently tailor electron-phonon interactions over picosecond time scales.

[1] Caruso, Novko, Draxl, Phys, Rev. B **101**, 035128 (2020).

[2] Novko, Caruso, Draxl, Cappelluti, Phys. Rev. Lett. **124**, 077001 (2020).

[3] Seiler, Zahn, Zacharias, Hildebrandt, Vasileiadis, Windsor, Qi, Carbogno, Draxl, Ernstorfer, Caruso, arXiv:2006.12873 (2020).

[4] Caruso, J. Phys. Chem. Lett. **12**, 1734 (2021).

Für diese Zeit steht eine Kinderbetreuung nach vorheriger Anmeldung zur Verfügung.

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