PHYSIKALISCHES KOLLOQUIUM

Sommersemester 2025

Das Kolloquium findet (soweit nicht anders angegeben) **jeweils montags um 14:15 Uhr in Präsenz im Röntgen-Hörsaal** des Physikalischen Instituts, Hubland Campus Süd, Universität Würzburg **und online via Zoom statt**.
Zugangsdaten siehe https://www.physik.uni-wuerzburg.de/aktuelles/veranstaltungen-aus-der-physik/physikalisches-kolloquium/

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Vorstellungsvortrag im Rahmen des Habilitationsverfahrens

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Making Molecular Movies - How Ultrafast Diffraction Captures Lattice Dynamics

Abstract

The crystal structure as well as the coupling of the electronic and lattice subsystems shape the thermal, optical and electronic properties of any material. While the optical and electrical properties are mostly governed by the electronic system, the lattice system reigns over the majority of thermal properties. The coupling between both mediates their energy exchange which, for example, determines loss channels and polaron formation during electric transport but also guides emerging phenomena such as charge-density wave transitions. While the dynamics of the electronic system are commonly probed by spectroscopic methods, there are complementary scattering techniques to probe the lattice dynamics.

In this talk, I will give an introduction into pump-probe diffraction experiments of crystalline samples with a focus on ultrafast electron diffraction (UED). I will review the scattering theory that serves as a basis to extract physical insights from the observables and discuss experimental challenges, the data analysis and sample preparation. I will show how UED can reveal complicated exciton-phonon coupling in complex materials such as molecular semiconductors. The size of the unit cell in these materials usually makes lattice dynamics and electron-phonon coupling inaccessible for ab-initio quantum chemical methods. In the case of the excimer, a molecular excited state that is energetically stabilized by a lattice distortion [1], the nuclear movement had to be indirectly inferred from spectroscopic techniques, so far. Using the instructive case of excimer formation in the molecular

semiconductor zinc-phthalocyanine [2], I will show how the excimer formation process can be directly followed by means of UED.

[1] Hammer S. et al., Mater. Horiz. 10 (2023), 221-234

[2] Hammer S. et al., PNAS 121 (2023), e2411975121

Für die Dozentinnen bzw. Dozenten der Fakultät

Prof. Dr. Hankiewicz, Prof. Dr. Hinkov, Dr. Meyer, Dr. Feichtner, Hr. Baumbach