

# Vortrag

## „Microscopic Theory of Structural Dynamics and Optoelectronic Properties of Halide Perovskites“

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#### Abstract:

Power-conversion efficiencies of solar cells based on halide perovskites (HaPs) have improved at a record speed and are currently above 22%, which pushed these systems to the forefront of materials, energy and nanoscience. It is both fundamentally and technologically important to understand phenomena that contribute to, or limit, the impressive optoelectronic performances of HaP-based devices. To this end, an ionic lattice displaced from static positions only by harmonic vibrations is typically invoked when examining charge-transport and light-absorption properties in the semiconducting material. However, a plethora of recent studies suggest that this picture is not sufficient for HaPs, in which different structurally dynamic effects, going strongly beyond small harmonic vibrations, occur already at room temperature.

After providing an introduction to HaPs and optoelectronic devices made from them, I will present our recent findings on the structural dynamics in HaPs, using density functional theory, molecular dynamics, multiphonon emission models and quantum-dynamics simulations. Starting from the canonical band structure picture, theoretical and experimental findings on the impact of low-energy optical phonons and dynamic polar distortions, driven by a mechanically soft lattice, will be discussed. Finally, I will demonstrate how the unusual structural dynamics in HaPs control their outstanding optoelectronic properties.