



PHYSIKALISCHES KOLLOQUIUM

des Fachbereichs Physik
der Johann Wolfgang Goethe-Universität Frankfurt

Mittwoch, den 20.12.2023, 16 Uhr c.t.
Großer Hörsaal, Raum _0.111,
Max-von-Laue-Str. 1



Prof. Dr. Irene Burghardt

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"Excitons at work in organic photovoltaics: Quantum dynamical simulations and 2D electronic spectroscopy"

The elementary steps of organic photovoltaics involve the conversion of excitons into free charge carriers, giving rise to a photocurrent. As highlighted by time-resolved spectroscopic observations, these elementary events often feature coherent transients, necessitating a description beyond conventional rate theories. In order to understand how coherent effects influence the transfer dynamics, and to what extent they are robust against static and dynamic disorder, quantum dynamical approaches are the method of choice. In this talk, we present a protocol that combines first-principles parametrized lattice Hamiltonians with accurate quantum dynamics simulations using advanced multiconfigurational methods. We show that this approach permits to resolve the subtle interplay of site-to-site transport, exciton and charge delocalization, and vibronic effects. Applications will focus on the molecular-level mechanism of exciton migration, singlet exciton fission, and exciton dissociation in regioregular donor-acceptor materials. We further present simulations of 2D electronic spectroscopy (2DES) signals that reveal the ultrafast signatures of these processes.

Die Dozenten der Physik

local host: Prof. Dr. Jens Bredenbeck | bredenbeck@biophysik.uni-frankfurt.de