

Donnerstag, 12.05.2022

Hörsaal D, Chemiezentralgebäude, 10:15 Uhr

**Sprecher:** **Caterina Cocchi**  
(*Universität Oldenburg*)

**Titel:** **Light-driven excitations in organic materials:  
Excitons, vibrations, and their coupled  
dynamics**

**Abstract:**

Light-matter couplings in organic materials lead to a rich landscape of electronic, optical, and vibrational excitations which closely depend on the characteristics of the systems (aggregation, functionalization, doping) as well as on the interactions with their environment. To address this complexity, *ab initio* methods such as (time-dependent) density-functional theory and many-body perturbation theory offer an ideal trade-off between accuracy and numerical complexity and can be successfully adopted to gain insight into different physical problems. In this seminar, I will present recent achievements of my group to this research area, where we contributed to better understand optical excitations in organic (co-)crystals [1-3] and donor/acceptor complexes [4,5], and to shed light into the fundamental mechanisms underlying the ultrafast response of organic molecules to coherent light, exciting both electronic and vibrational degrees of freedom [6-9].

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**Organisation: B. Engels**