

Seminář Fyzikálního ústavu UK

Úterý 13. 10. 2026

Ateliér Fyzikálního ústavu UK

Ke Karlovu 5, Praha 2, 2. patro po schodech na konci chodby.

ve 14:00 hod

Structure based modelling of exciton-exciton annihilation

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In my seminar, I will introduce my new research project, which focuses on developing a structure-based model to simulate and understand exciton–exciton annihilation (EEA) in photoactive materials. EEA is an important loss mechanism that can limit the performance of many photoactive devices, including solar cells, lasers, and light-emitting diodes, particularly at high exciton densities. At the same time, EEA can be beneficial in certain applications, for example by facilitating charge generation in organic semiconductors and solar-cell materials. Currently, modelling of EEA is largely based on quantum master equations or diffusion-based formalisms with (semi-)empirically fitted parameters. While these approaches can successfully describe experimental observations, they provide limited insight into the relationship between molecular structure and EEA dynamics and have limited predictive capability for new materials. The primary objective of the project is to develop a structure-based framework for EEA in which the relevant parameters are calculated directly from molecular structures using ab initio electronic-structure methods and open-quantum-system approaches. Connecting molecular structure directly to exciton dynamics will provide a route towards understanding and ultimately designing materials with tailored EEA properties for next-generation optoelectronic applications. I will present the main concepts behind the project, the key challenges, and our preliminary results.