INVITATION

Department of Condensed Matter Physics

Is pleased to invite you to the lecture

Structure-property relationship in binary blends: Tuning the photophysics of molecular materials

by

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One of the fundamental questions in condensed matter is that of the structure-property relationship, which we will discuss using molecular materials. Pentacene (PEN) is the prototypical small-molecule semiconductor, even exhibiting singlet fission (SF).
Here we present a comprehensive investigation how the photophysics of PEN can be tuned in binary blends (PEN:XXX).
To this end, we study a wide range of systems PEN:XXX with different structural motifs and different levels of coupling of XXX (=DIP, 5PH, 6PH, TIPS-PEN, TET, 3P, C60, ADT, HEX, DNTT) with PEN. These include unconventional structural motifs, such as a frozen-smectic structure, as well as different levels of phase separation vs. intermixing / solid solutions and co-crystal formation.
The resulting optical properties range from “dissolution” of PEN in picene (PIC) and robust SF (Broch et al., Nature Commun. 9 (2018) 954) to strong coupling and charge transfer (CT) with perfluorinated PEN (PFP) and essentially all scenarios in between.
Importantly, even for the case of intermixing, the local structure can strongly impact the resulting optical spectra, implying that it is not sufficient to know the global mixing behavior, as demonstrated for PEN:TET (Unger et al., J. Phys. Chem. A 128 (2024) 747)
We will finish with an outlook on possible future steps, including the study of molecular dynamics using XPCS (X-ray photon correlation spectroscopy; Dax et al., New J. Phys. 23 (2023) 103033) and strategies to make these studies more efficient by high-throughput and machine learning techniques (Hinderhofer, J. Appl. Cryst. 56 (2023) 3; Lapkin, in preparation).
Contributions by numerous students and external collaborators are gratefully acknowledged.

Date: **2 October 2024**

Time: **11:00**

Venue: **Lecture room F1, Building 6, Faculty of Science, Kotlářská 2, Brno**

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