FACOLTÀ DI SCIENZE MATEMATICHE, FISICHE E NATURALI
DIPARTIMENTO DI MATEMATICA E FISICA "NICCOLÒ TARTAGLIA"

Modifying intermolecular interactions in acenes: The impact on Davydov-splitting and singlet fission

Introduce:
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Abstract
Singlet fission, which is the photophysical process in which an excited singlet state on one molecule is transformed into two excited triplet states on neighboring molecules, has the potential to significantly boost solar cell efficiencies [1,2] and, thus, has received increasing attention in the last decade.
One research focus lies on the impact of intermolecular interactions and (virtual or real) charge transfer states on singlet fission [3,4] as a possible way towards the synthesis of singlet fission capable organic molecules. However, the details of the interplay between interaction strength and singlet fission efficiencies are still unclear [5]. To obtain further insight into these mechanisms, the targeted modification of intermolecular interactions is a promising approach. So far, this is mainly achieved via side chain modification [4,5] or in chemically linked dimers [6]. Both approaches have advantages as well as disadvantages, such as the need for complex chemical synthesis.
The talk will discuss an alternative approach which is based on the coevaporation of the singlet fission material with a weakly interacting spacer compound [7]. This leads to the formation of mixed films with well-defined long range order and reduced intermolecular interactions, which can be tuned easily over a wide range and for which the Davydov-splitting is a convenient metric [8].
The impact of the modification of intermolecular interactions on singlet fission time constants will be discussed using the examples of pentacene and tetracene.

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Seminario

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