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Promotionsverfahren von **Herrn M.Sc. Simon Hédé**
Auslage der Dissertation und Gutachten sowie Termin der mündlichen Prüfung
Anlage: Einseitige Zusammenfassung der Dissertation

Sehr geehrte Damen und Herren,

in dem oben genannten Promotionsverfahren wird die Annahme der Dissertation

Influence of complex environments on the photophysical properties of organic chromophores.

von den Berichterstattenden PD Dr. O. Weingart und Prof. Dr. C. Janiak beantragt. Sie kann zusammen mit
den Gutachten in der Zeit

vom 02.12.2024 bis 11.12.2024

eingesehen werden. Bitte wenden Sie sich zur Einsicht an das Promotionsbüro (promotionmnf@hhu.de).

Einsprüche gegen diese Dissertation können nur zwei Tage nach der vorgenannten Frist
geltend gemacht werden. Erfolgt kein Einspruch, so gilt die Dissertation als angenommen
(§ 7 Ziffer (5) PO).

Sofern die Dissertation angenommen wird, findet die mündliche Prüfung am

16.12.2024 um 15.30 Uhr

im **Hörsaal 6C** statt. Als Prüferinnen bzw. Prüfer sind vorgesehen:
Prof. Dr. C. Marian, Juniorprof. Dr. J. Meisner und Juniorprof. Dr. M. Suta.

Die Öffentlichkeit ist bei der Befragung nicht zugelassen.

Mit freundlichen Grüßen
im Auftrag

Daniela Schleiffer

Abstract

In this thesis, a protocol to compute the photophysical properties of chromophores within complex solid state embedding was established and validated. The protocol involves plane wave calculation of experimentally obtained crystal structures and subsequent QM/MM calculations centred on one or multiple chromophores. The use of a QM/MM scheme allows the inclusion of explicit surroundings that would be impossible to study solely relying on quantum mechanical based methods.

The first study was conducted on the effect of three different environments on the MIA chromophore, involving the MIA organic single crystal and two MOFs. This experiment illustrated the significance of including inter-molecular interactions to describe electronic properties in a condensed medium. In the MIA single crystal, the first excited state corresponds to a charge transfer between neighbouring MIA molecules, while both MOF structures basically prevent aggregation and interaction of chromophores by isolating them.

A second study was conducted on three different (co-)crystals based on a flavin derivative. The co-crystals modify the emission wavelength of the flavine. The performed QM/MM computations could explain the reasons behind experimentally observed blue-shifts in emission. The distance between the molecules involved in the charge transfer has a major effect: the larger the distance, the more the emission shifts to smaller wavelengths. The type of in-plane neighbours also weakly affects the emission.

In the third study, three phenazine derivatives were investigated as potential TADF emitters in solvent and in their own single crystal. Calculations on these models were at first performed using standard methods but led to inadequate results. By introducing vibrational effects into the calculation, I was able to identify TADF in two of the three molecules, matching the experimental observations. The difference between solvent and crystalline medium on the TADF properties could also be assessed.

The last study presented in this thesis aimed at investigating singlet fission in pentacene and TIPS-pentacene in their single crystal environment. The application of the here established protocol helped in identifying the mechanism of the singlet fission process, which was only achievable due to detailed description of the crystal embedding.