PhD Open Seminar

Department of Chemistry, IISER Bhopal

Title of Thesis: **Functionalized Perylene and Terrylene Diimide Derivatives for Panchromatic Absorption: Synthesis, Structure and Properties**

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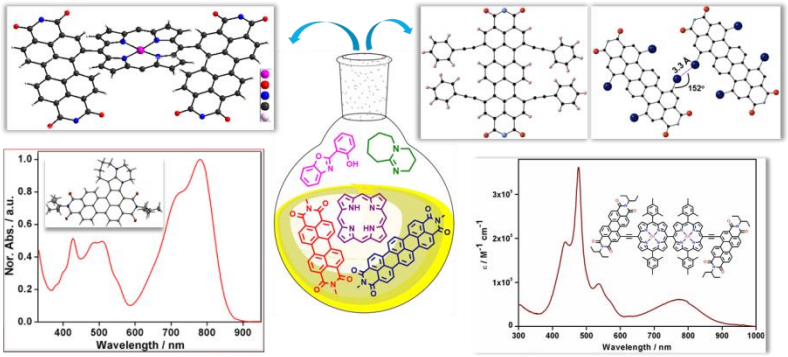
Abstract

Perylene diimides (PDIs) and terrylene diimides (TDIs) are popular n-type semiconducting materials. Functionalized PDI derivatives were explored for emerging applications in the field of organic photovoltaics, organic field-effect transistors, bio-labelling, and supramolecular assemblies. While PDIs have been studied intensively, the higher homologues such as TDIs were less explored. This is due to the challenging synthesis and poor solubility originating from strong π-π stacking making the synthesis, processing and characterization of this class of molecules rather difficult.[1]

In this thesis, we have presented different synthetic strategies and functionalities of PDI and TDI derivatives. We demonstrated the synthesis and photophysical properties of several directly-connected perylene diimide-porphyrins (PDI-POR) based push-pull systems.[2] Then, the reactivity of 1,8-diazabicyclo[5,4,0]-undec-7-ene (DBU) towards various perylene derivatives were explored and the resultant new chromophores were identified as semi-coronene diimide (sCDI), pyrrolo-PDI (pPDI) and DBU-annulated-PDI (PDIDBU) derivatives and their optical properties were investigated.[3] Further, the *bay*-functionalization of TDIs resulted in near infra-red (NIR) absorbing as well as emitting core-twisted TDI derivatives.[4] Then, the optical properties of 2-[2'-(Hydroxyphenyl)]benzoxazole (HBO) substituted PDI derivatives were demonstrated towards ESIPT property.[5] Some of the PDI derivatives were utilized as donor materials in bulk-heterojunction organic solar cells (BHJ-OSCs) application.[6]



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[2] (a) Mishra, R.; **Regar, R.**; Singhal, R.; Panini, P.; Sharma, G. D.; Sankar, J. *J. Mater. Chem. A* **2017**, *5*, 15529; (b) **Regar, R.**; Sankar, J. (Unpublished results); (c) **Regar, R.**; Sankar, J. (Manuscript under preparation).
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[4] (a) **Regar, R.**; Mehra, K. S.; Bhowal, R.; Sankar, J. *Eur. J. Org. Chem*. **2019**, *36*, 6278; (b) **Regar, R.**; Sankar, J. (Unpublished).
[5] **Regar, R.**; Sankar, J.; Ulrich, G. (Unpublished).
[6] **Regar, R.**; Mishra, R.; Singhal, R.; Sharma, G. D.; Sankar, J. *J. Mater. Chem. A* **2019**, *7*, 3012.