ITI HiFunMat Master Internship Proposal

☐ M 1 ☒ M 2

Title: Liquid crystals in Small-molecule Organic Solar Cells: a new approach to higher efficiency

Internship supervisor

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Laboratory	ICube
Collaboration with a HiFunMat member (*please indicate their name*)	☐ No ☒ Yes : Thomas Heiser, ICube

Student profile looked for

Master program (*more than one box can be ticked)*	☒ Material science and engineering ☐ Chemistry ☒ Physics
Other indications if necessary	

Internship description

For sustainable global economic growth, an abundant supply of energy is essential. At the same time, our energy needs are increasing in order to improve our lives. In the long run, the supply of conventional energy is limited, and will not be able to meet future energy demand. To solve the global energy crisis, the development of solar energy is undoubtedly one of the best answers. Despite development in inorganic photovoltaic device, organic photovoltaics remain a promising low-cost renewable energy technology, due to the versatility of organic semiconductor materials and simple device structures that can be constructed by a variety of printing techniques. Recently, organic solar cells with polymer as donors have achieved excellent efficiencies over 18%. Compared with polymers, small molecules seem to be more promising because of their high purity, well-defined molecular structure and reproducibility in organic solar cells (OSCs). However, the power conversion efficiencies (PCEs) of small molecule donors currently still lag behind their polymer-based counterparts, which is usually limited by their relatively the phase separation morphology of the active layer. Typically, the ideal morphology implies reasonable molecular crystallinity and large correlation scales, which favour excitons, separation, and charge transport. To improve the morphology, a new concept has been recently investigated, by introducing of liquid crystals (LCs) in the organic materials. According to the literature, the good exciton diffusion length and the high charge-carrier mobility of discotic (disc-shaped) liquid crystals lead to a high efficiency organic photovoltaic solar cells.[1] Most recently, J. Wen reported ternary OSCs based on a broad-band donor polymer and a low-band acceptor system. The introduction of a calamitic (rod-like) liquid crystal donor results in an efficiency of up to 17.92%.[2]

This internship aims to explore this approach in small-molecule (SM) OSCs, understand the mechanisms underlying the interactions between LC molecules and small molecules donor/acceptor. We will investigate the influence of the molecular shape of LCs of physical, optical, and electrical proprieties of the new mixture of active layer. The final goal is to obtain a high efficiency SM OSC.

References:
[1] Zheng Q. et al., Efficiency improvement in organic solar cells by inserting a discotic liquid crystal. Sol. Energy Mater Sol. Cells, 95,2200-2205 (2011).
[2] Wen J. et al., Efficient and Stable Ternary Organic Solar Cells Using Liquid Crystal Small Molecules with Multiple Synergies. ACS Appl. Energy Mater. 5, 12809–12816 (2022)