ITI HiFunMat Master Internship Proposal

☐ M 1 ☒ M 2

Title: Sustainable Solvents For High-Performance Organic Solar Cells By Reverse Engineering

Internship supervisor

Name, first name	Heiser Thomas
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Laboratory	ICUBE
Collaboration with a HiFunMat member (*please indicate their name*)	☐ No ☒ Yes : Patrick Lévêque, Yaochen Lin

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

Scientific Context

For a sustainable scale-up of solution-processed organic photovoltaic modules, the replacement of toxic solvents by alternative "green" solvents, which minimize the environmental impact and pose no risk to human health, is a critical issue. Yet, because of the complex relationship between the solvent properties and the device performances, the selection of alternative solvents most often relies on time-consuming and costly trial-and-error approaches. A more efficient and less empirical method to identify green solvents, based on a reverse engineering approach, has recently been proposed by our project consortium.[1,2] The method starts by specifying the requested physico-chemical properties of the target solvent and utilizes a genetic algorithm, combined with the modeling of critical molecular properties, to identify potentially new solvents. The candidate solvents are ranked as a function of a global performance factor, which specifies how the estimated properties compare to the target values.

The initial application of this method to select alternative solvents for the fabrication of organic solar cells has produced promising results. However, the molecular property estimation tool was originally based on a group contribution method, which limits result accuracy. Recently, a more advanced modeling approach, COSMO-RS (COnductor-like Screening MOdel for Real Solvents), was implemented, significantly enhancing the relevance of the solvent performance factor.

The objective of this internship is to experimentally evaluate the performance of alternative solvents identified using the enhanced reverse engineering method. This project will be conducted in close collaboration with Professor Ivonne Rodriguez's team (Laboratoire de Chimie Agro-Industrielle at INP Toulouse), where the reverse engineering technique is applied. The focus will be on depositing and characterizing thin films of cutting-edge organic photovoltaic blends formulated with the new eco-friendly solvents. The top-performing solution will then be used to fabricate and analyze organic solar cells.

References:
[1] J. Wang et al, Mol. Syst. Des. Eng., 2022, 7, 182
[2] Projet ANR/DFG GreenPhotoSolv, ANR-21-CE05-0031

Requirements & Application

We are seeking a motivated master's student with a strong interest in organic photovoltaics, eager to learn about wet thin film deposition of organic semiconductors, as well as fabrication and characterization (optical and electrical) of organic devices.

Please address your application including a CV, a motivation letter and Master transcript of records to Thomas HEISER and Yaochen LIN, Laboratoire ICUBE.

Possible starting date : Jan- February 2025

***Note that the lab is within a ZRR (Zone à Régime Restrictive)**