ITI HiFunMat Master Internship Proposal

☐ M 1 ☒ M 2

Title: Atomic scale simulation of exciton dynamics in organic materials for photovoltaic applications

Internship supervisor

Name, first name	Martin, Evelyne
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Laboratory	ICube
Collaboration with a HiFunMat member (*please indicate their name*)	☐ No ☒ Yes : Steveler, Emilie and Heiser, Thomas

Student profile looked for

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

Internship description

In organic solar cells, light is absorbed and generates a bound electron-hole pair, i.e. an exciton, in a polymer or small molecule. The photogenerated exciton diffuses until it dissociates at the interface between electron-donor and electron-acceptor materials into two free particles, an electron and a hole, that are collected and create an electric current. The modeling of the exciton diffusion and dissociation enables the understanding of its atomic-scale origin, and will allow in fine to optimize the devices and increase their efficiency.

The purpose of the internship is to study the exciton diffusion by resorting to an atomic scale method that describes both the ionic and electronic motion, i.e. first-principles molecular dynamics (FPMD). Recently, we have proposed and published a FPMD-based methodology able to predict the measured diffusion coefficient in the P3HT polymer, a donor photovoltaic material widely characterized. The purpose of the internship is to learn the computational methodology and apply it to an acceptor molecule in order to achieve a deeper understanding of the exciton life and recombination.

The candidate will interact with the PhD student who did the calculation on the P3HT, and more globally with the students and researchers of the modeling consortium ADYNMAT . He will also interact with the members of the organic electronics consortium STELORG.

Daily work will be performed on the computer. Skills in materials physics/chemistry are expected (electronic structure, thermodynamics).