A nanoscale approach of fundamental processes in photovoltaic cells

DIRECTEUR DE THESE : JEAN-PIERRE BUCHER
EQUIPE ASSOCIEE A L'IPCMS, UNIVERSITE DE STRASBOURG
TEL : 03 88 10 70 96 ; E-MAIL : JEAN-PIERRE.BUCHER@IPCMS.UNISTRA.FR

Organic photovoltaic cells consisting of donor (D) and acceptor (A) layers have been regarded as the next-generation of hetero-junction organic solar cells mainly because they possess fascinating advantages, such as low fabrication cost, lightness, and flexibility, when compared to more conventional devices based on semiconductor compounds [1]. It is the purpose of this PhD project to get a better understanding of the correlation between the external quantum efficiency (EQE) and nano-structural properties such as molecular orientation, crystallinity, D/A interface, for improving the energy conversion efficiency η. Any combination of D and A molecules will be studied *in situ* on a substrate by means of ultrahigh vacuum (UHV) scanning tunneling microscopy/spectroscopy (STM/STS) at liquid helium temperature (T=4.6 K) [2]. The electronic intermolecular states as well as the spectroscopic data on the onset of HOMO and LUMO state on both A and D molecules in the different configurations will be studied in detail. Comparison of STS spectra with first-principle calculations will be made to clarify (1) whether or not intermolecular charge-transferred exciton states are formed between adjacent D-D and A-A molecules and (2) whether or not a localized band-bending (polarization) close to the D-A interface is taking place.

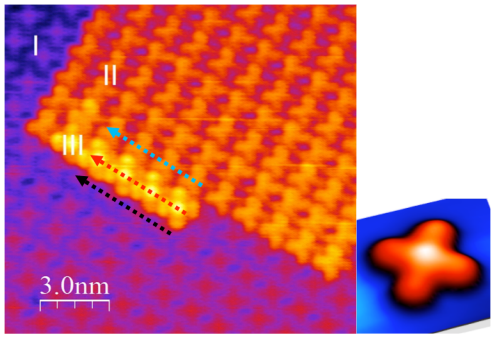

Figure 1: STM image of first, second and third layer phthalocyanine molecules grown under UHV on Ag(111) and studied at T= 4.6 K. Inset : isolated molecule.

The candidate will be involved in a collaborative project in which the EQE of organic solar cells will be examined macroscopically the using *in situ* electrical field modulated spectroscopy under UHV [3]. For the purpose of this work, hetero-junctions of donor (phtharocyanine or porphyrin) and acceptor (C_{60}) films characterized by XRD/SEM/TEM will be used [3,4]. Other molecules with specific ligands that are synthesized on demand by our collaborators will be used as well. We are looking for a highly motivated candidate with a scientific master degree. He/she should have a good background in physics and material science. The candidate will have the opportunity to participate in an international pluridisciplinary exchange program with Japan.

1. H.-Y.Chen et al. *Nat. Photonics* **3** 649 (2009) & Y. Liang et al. *Adv. Mater*. **22**, 135 (2010).
2. S. Kezilebieke et al. *Nano Research*, **7**, 888 (2014); A. Amokrane et al. *J. Phys. Chem. Lett*. **5**, 3175 (2014).
3. S. Ryuzaki et al. *Nano Rev.* **4**, 21055 (2013) & *J. Phys. D*: *Appl. Phys.* **44**, 145103 (2011).
4. M. Nakaya et al. *ACS Nano* **8**, 12259-12264 (2014).