UCL Université catholique de Louvain

IMCN Institut de la matière condensée et des nanosciences

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SEMINAR

«Identification of Next-Generation Materials for Organic Solar Cells via a Collaborative Theory-Experimental approach »

Monday 17 October 2016 – 14:00
LAVO51 – Lavoisier - Place L. Pasteur, 1, – LLN

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ABSTRACT

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Today's global energy expenditure is dominated by non-renewable energy sources (*i.e.* fossil fuels). The entire global energy demand is several orders of magnitude smaller than that of solar energy received by the Earth. Photovoltaics represent a possible solution to harness this plentiful resource and transform our energy budget and offset global warming. An array of photovoltaic technologies is needed to utilize this vast resource; thin-film organic photovoltaics (OPVs), made from low-cost carbon-based materials, are finding use in building-integrated PV (BIPV) systems, flexible power generation systems, and many other niche markets.

Our efforts are focused on OPVs, which require a donor and an acceptor material to facilitate exciton dissociation into free charge-carriers. This presentation will describe two instances of *in silico* screening utilizing the *Harvard Clean Energy Project* to discover new non-fullerene acceptor materials. The first part of the presentation will introduce non-fullerene acceptors and describe how *in silico* screening studies are carried out. I will present unpublished preliminary results stemming from a large theoretical screening (56,000 potential acceptor materials) and a smaller screening (~100 potential acceptor materials) theory-experiment collaboration with the Loo group (Princeton University) has demonstrated the dual utility of these approaches.

We utilized a variety of quantum mechanical calculations using density functional theory (DFT) and time-dependent density functional theory (TD-DFT) to evaluate the electronic structure of contorted electron donor and acceptor materials to guide the next generation of materials using the combined expertise of our groups. The excitation energies (and likely electronic transitions) were computed to determine materials capable of efficiently absorbing solar photons. Taken together, a new series of donor-acceptor pairs were identified, and are currently being synthesized.

BIOGRAPHY

Education

- Doctorate in organic chemistry (PhD): University of California, Los Angeles, 2010-2015. Advisor: Kendall N. Houk
- Bachelor of Science in chemistry (BS): New York University, New York, NY, 2006-2010

Research interests:

- Organic Photovoltaics
- Crystal Structure Prediction
- High-throughput in-silico screening
- QM/MM modeling of OPV interfaces
- Electronic processes at BHJ interfaces

The pubications are available on http://aspuru.chem.harvard.edu/steven-lopez/