CORE-CM SEMINAR
Michigan State University

Timothy P. Bender
University of Toronto

Non-Fullerene Electron Accepting Materials in Organic Photovoltaics: synthesis, device engineering and lifetime assessments

For some time, our group has been focused on the design and synthesis of derivatives of boron subphthalocyanine (BsubPc). Our focal point is equally between the basic chemistry of BsubPcs and their application in organic electronics. We do focus on two specific device applications, organic photovoltaics (OPVs) solar cells and organic light emitting diodes (OLEDs).

I will begin by presenting our efforts with regards to synthetic variants of BsubPcs and their application in planar heterojunction (PHJ) OPVs.[1,2] I will then outline our very recent results where we took BsubPc based PHJ OPVs for real time roof testing. What we found was that when BsubPcs are applied as electron accepting materials they are remarkably stable and maintain 4-6% PCE over time. On the flipside, when applied as electron donating materials the stability of the paired material, C_{60}, fullerene, dictates the overall stability of the devices. Moreover, we have used a novel method to map out the degradation pathway of the OPVs which will be described. We were able to ultimately form a structure property relationship to their stability in the ambient environment. These results and past data on the harvesting of triplet from pentacene via BsubPcs, has led us towards additional BsubPc derivatives with peripheral halogenation which will be outlined. In addition, we recently began the exploration of the bulk-heterojunction (BHJ) OPV space utilizing BsubPcs as an electron accepting fullerene alternatives.[3,4]

In parallel we have also been exploring the concept of complementary absorption engineering by either the chemical modification of BsubPcs or by pairing BsubPcs with alternative materials having complementary absorption profiles. For example, we have recently shown that after firming up the chemical structure of phosphorus oxy tetrabenzotriazacorrole [POTbc, a phthalocyanine analogue] that the pairing of a BsubPc with POTbc yields a unique gray organic photovoltaic cell absorbing broadly across the visible spectrum.

We have also recently shown that structural analogs to BsubPcs, boron subnaphthalocyanines (BsubNcs) are actually a mixed alloy composition of chlorinated materials designated as Cl-Cl_nBsubNcs. After establishing the correlation of electrochemical characteristics and OPV performance for Cl-Cl_nBsubNc we have described how phenoxylated versions of Cl_nBsubNc are as well applicable in BHJ OPVs as electron accepting materials. Furthermore, we have explored the potential of chemistry variations to yield pure examples of BsubNcs. Time permitting this will be outlined along with electrochemical characterization and the exploration of alternative synthetic pathways to BsubNcs that do not yield mixed alloyed materials.

The final topic that I will present is the exploration of additional p-block metal phthalocyanines (Pcs); we came to conclusion that silicon phthalocyanines (SiPcs) can also be applied as fullerene alternatives/acceptors in organic photovoltaic cells. Over the past year we have formed an initial structure property relationship that gives a road map to synthetic alternatives of SiPcs that have the potential to yield higher performing OPVs (in both PHJ and BHJ structures). Finally I will show how a SiPc is actually equivalent to the most studied fullerene ($PC_{61}BM$) in many metrics including power conversion efficiency in OPVs.

Coauthors and coinvestigators will be cited as appropriate throughout the presentation.

References:

[1] Cnops, K.; et al., *Nature Comm.*, 5, Article number: 3406, DOI:10.1038/ncomms4406.
[2] Verreet, B.; et al., *Adv. Energy Mater.* 2014, 1301413, DOI:10.1002/aenm.201301413.
[2] Ebenhoch, B.; et al., *J. Mater. Chem. A*, 2015, 3, 7345. DOI:10.1039/C5TA00715A
[3] Duan, C.; et al., *Angew. Chem. Int. Ed.*, 2016, DOI: 10.1002/anie.201608644.

Thursday, November 15, 2018 - 12:00 NOON
Room 1400 – Biomedical & Physical Sciences
Professor Annick Anctil– Host
Eunsang Lee - Student Host