

NSERC CREATE  
  
**TOP-SET**

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Séminaire

Le vendredi 15 décembre 2017, 15h30  
Des rafraîchissements seront servis dès 15h  
Complexe de recherche avancée, pièce 233  
Université d'Ottawa, 25, rue Templeton

\*Le séminaire se déroulera en anglais.\*

Seminar

Friday, December 15, 2017, 3:30 p.m.  
Refreshments to be served starting at 3 p.m  
Advanced Research Complex, room 233  
University of Ottawa, 25 Templeton Street

**Non-Fullerene Electron Accepting Materials in Organic Photovoltaics:  
Synthesis, Device Engineering and Lifetime Assessments**

**Timothy P. Bender, University of Toronto**

**Abstract:** 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. 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<sub>60</sub>, 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.

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<sub>n</sub>BsubNcs. After establishing the correlation of electrochemical characteristics and OPV performance for Cl-Cl<sub>n</sub>BsubNc we have described how phenoxyated versions of Cl<sub>n</sub>BsubNc 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.

**Bio:** Since his appointment at the University of Toronto in 2006, **Timothy P. Bender's** laboratory has focused on the design, synthesis and engineering of new materials for application in organic electronic devices including organic photovoltaics (OPVs) and organic light emitting diodes (OLEDs). His focus has been on two distinctly different classes of materials. The first is the development of the chemistry, crystal engineering and application of boron subphthalocyanines (BsubPcs) and related phthalocyanines (Pcs). The second is the design and application of soft or liquid triaryl amines. Permeating through each research stream is an interest in developing and studying polymeric versions of each class of material. Professor Bender's research contributions span from fundamental aspects of chemistry, to applied chemistry to physical chemistry and to the study of basic optoelectronic properties of organic electronic materials within organic electronic devices. Since 2006, he has published over 60 papers largely in peer reviewed high impact journals. He has active collaborations with a number of academic and industrial partners from the U.K. and the U.S. Professor Bender is a full professor cross-appointed to the Departments of Chemistry and Materials Science and Engineering at the University of Toronto and in 2016 was appointed as Associate Chair of his department in charge of the accredited undergraduate Chemical Engineering program. His research program at the University of Toronto is in part an extension of his independent research carried out while being a member of the research staff of Xerox Research Centre of Canada (2000 – 2006). During that time he was issued 60 US patents and published 5 peer reviewed articles primarily in the field of organic electronic materials with a focus on OLEDs and organic photoreceptors – the heart of a modern xerographic print engine. His inventions include novel blue-wavelength photoresponsive materials and a sol-gel based hole-transporting material the latter of which was taken to commercial production an enabled the photoreceptor to be a so called 'life of machine' part.



**TOP-SET** est un programme de formation FONCER du CRSNG en puissance optoélectronique ayant pour but de façonner une cohorte de personnel hautement qualifié détenant des connaissances approfondies en systèmes optoélectroniques pour joindre les rangs d'équipes de recherche et développement.

NSERC CREATE Training in Optoelectronics for Power: from Science and Engineering to Technology (**TOP-SET**) is a training program that aims to form a cohort of highly qualified personnel with comprehensive understanding of optoelectronic systems, capable of joining advanced R&D teams.

Pour de plus amples renseignements sur TOP-SET, veuillez contacter Christine Couture, [sunlabadmin@uottawa.ca](mailto:sunlabadmin@uottawa.ca)

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