Canadian Association of Physicists | Association canadienne des physiciens et physiciennes

Contribution ID: **1542** Type: **Poster (Student, Not in Competition) / Affiche (Étudiant(e), pas dans la compétition)**

POS-19 - A DFT Investigation of Conjugated Polymers/Oligomers and Fullerenes Interactions in Bulk Heterojunction Organic Solar Cells

Wednesday, 31 May 2017 18:00 (2 minutes)

The performance of bulk heterojunction organic solar cells made of conjugated polymers/oligomers and fullerenes has significantly improved in the last few years (with PCE exceeding 10%).1 Experiments suggest that the intermolecular interactions between polymers and fullerenes are critical to the design of (even) more efficient organic photovoltaic cells.2 However, a detailed understanding of these intermolecular interactions is still lacking. In this work, we employ dispersion corrected density functional theory (DFT) methods, wB97xD, B3LYP-D3, B97D3, and PBE1PBE-D3, to investigate the properties of these heterogenous interactions in various promising oligomer/fullerene combinations (e.g. a pair of PC71BM and a copolymer based on thieno[3,4-b]thiophene/benzodithiophene (PTB7)3, PCBM and a copolymer based on 2,7-carbazole/dithienyl-2,1,3-benzothiazole (PCDTBT)4, and PC71BM and a copolymer based on difluorobenzothiadizole/quaterthiophene (PffBT4T-2OD)1). In particular, we determine and analyze the conformational and electronic structures, and binding energies of these combinations. We obtain the most preferred orientations of oligomers with respect to fullerenes and analyze the connection between their electronic structures and device performances. Finally, using binding energies, we assess the strength and stability of the oligomer/fullerene intermolecular interactions.

Keywords: Polymer/Fullerene Interactions, Organic Solar Cells, DFT.

[1] LIU, Y., ZHAO J., LI, Z., et al. 2014. Nature Communications.
[2] HUANG, Y., KRAMER, E., HEEGER, E., et al. 2014. Chemical Reviews.
[3] HE, Z., ZHONG, C., SU, S., et al. 2012. Nature Photonics.
[4] BEAUPR´E, S. & LECLERC, M. 2013. Journals of Materials Chemistry.

Primary authors: AYOUB, Sarah (Memorial University); LAGOWSKI, Jolanta (Memorial University of Newfoundland)

Presenters: AYOUB, Sarah (Memorial University); LAGOWSKI, Jolanta (Memorial University of Newfoundland)

Session Classification: DCMMP Poster Session | Session d'affiches DPMCM (9)

Track Classification: Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)