Contribution ID: **86** Type: **Talk**

Toward the rational design of organic solar photovoltaics: Application of molecular structure methods to donor polymers

Conjugated polymers are promising candidates in the design of polymer solar cell materials with suitable electronic properties. Recent studies show that the use of different functional groups as side chain substitutes in thiophene-based polymers changes the electronic and conformation structures. Here we design new thiophene based molecules by replacing the hydrogen attached to the backbone of P3MT with electron donating and electron withdrawing groups. We then calculate the HOMO, LUMO, HOMO-LUMO energy gap to quantify the theoretical merit of the new polymers as solar absorbers and their inter-ring torsional potential to understand their suitability to link together in high conductivity, extended conjugated systems. Calculations are done with first principles density functional theory (DFT), implemented using B3LYP with dispersion function and 6-31G(d, p) as basis set. Our calculations show a possible approach to the rational design of donor materials when substituents are inserted systematically in a generic oligomer.

Student?

No

Supervisor name

Supervisor email

Primary author: Prof. PELLICANE, Giuseppe (University of KwaZulu-Natal)

Co-authors: MAMBA, Sandile (University of Kwazulu Natal); Prof. PERRY, David (University of Akron); Prof. TSIGE, Mesfin (University of Akron)

Presenter: Prof. PELLICANE, Giuseppe (University of KwaZulu-Natal)

Session Classification: HPC Applications

Track Classification: Materials Science