Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Small Conjugated Molecules: Orbital Energy Modeling Using Tuned Range-Separated Functional[1] RAM BHATTA, MESFIN TSIGE, Department of Polymer Science, The University of Akron — Small conjugated molecules (SCMs) have potential to be efficient electron donors for organic solar cells because of their structural simplicity, good control over synthetic reproducibility and low purification cost. Density functional theory (DFT) and time dependent DFT (TDDFT) computations can guide for designing high-performing SCMs by modeling their orbital energies. However, the accuracy of computed orbital energies depends on the choice of the level of the theory. We present DFT and TDDFT calculations on 12 different SCMs using range-separated functional, LC-BLYP and the popular hybrid functional, B3LYP. Systematic calculations of the highest occupied molecular orbital (HOMO) energies, the lowest unoccupied molecular orbital (LUMO) energies as well as the singlet and triplet excitation energies are performed. We found that the LC-BLYP results are strongly dependent on the range-separation parameter. The computed results are compared with experimental data.

[1]Work supported by the National Science Foundation (Grant No. DMR0847580)

Ram Bhatta
Department of Polymer Science, The University of Akron

Date submitted: 14 Nov 2014 Electronic form version 1.4