RESPONSE TO REVIEWER

Reviewer # 1:

Thank you for your review and valuable recommendation. The paper has been revised according to your comments with following clarifications:

Comment1 In table 1, the authors mention about bond length. Unfortunately, the authors did not mention that bond length is the bond length between atom ... and atom ...

Response: Table1 shows root mean square deviations (RMSD) of bond lengths of optimized Py structures (n= 1 to 5 units) by B3LYP/3-21G* and SCC-DFTB comparing with B3LYP/6-31G*. They are not bond length values. The RMSD values were calculated by a simple equation; for example of RMSD of SCC-DFTB, $RMSD = \sqrt{\frac{\sum(X_{DFTB} - X_{B3LYP})^2}{n}}$, where X_{DFTB} and X_{B3LYP} are structural properties obtained by SCC-DFTB and B3LYP/6-31G* methods, respectively.

Comment2 The bond length in table on is unreasonable. Typically, the bond length of atom is in unit of Angstrom. For example, hydrogen bond length is roughly 0.5 Angstrom. The bond length in table 1 is in order of milli angstrom !!!

Response: They are not bond length values. Table1 shows root mean square deviations (RMSD) of bond lengths of optimized Py structures (n= 1 to 5 units) by B3LYP/3-21G* and SCC-DFTB comparing with B3LYP/6-31G*. Full list of geometries parameters of PPy oligomers is summarized in Table S1 of the supplementary data section.

Comment3 In table 1, the authors mention did not mention that bond angle is the bond angle between atom ... and atom ...

Response: Table1 shows root mean square deviations (RMSD) of bond angles of optimized Py structures (n= 1 to 5 units) by B3LYP/3-21G* and SCC-DFTB comparing with B3LYP/6-31G*. They are not bond angle values. The RMSD values were calculated by a simple equation; $RMSD = \sqrt{\frac{\sum(X_{DFTB} - X_{B3LYP})^2}{n}}$, where X_{DFTB} and X_{B3LYP} are structural properties obtained by SCC-DFTB and B3LYP/6-31G* methods, respectively.

Comment4 The authors said the bond length, bond angle and torsion angle do not change significantly with increasing oligomers up to 5 units. If I understand correctly, the bond angle with n=5 is 1.001 degree in B3LYP/3-21G* method, but the the bond angle with n=5 is 0.507 degree in SCC-DFTB method. It is about 2 times or nearly 100% difference! Basically, we don't call it "do not change significantly"

Response: They are not bond length, bond angle and torsion angle values. Table1 shows root mean square deviations (RMSD) of structural properties including bond lengths, bond angle and torsion angle of optimized Py structures structures (n= 1 to 5 units) by B3LYP/3-21G* and SCC-DFTB comparing with B3LYP/6-31G*. The RMSD values were calculated by a simple equation; $RMSD = \sqrt{\frac{\sum(X_{DFTB} - X_{B3LYP})^2}{n}}$, where X_{DFTB} and X_{B3LYP} are structural properties obtained by SCC-DFTB and B3LYP/6-31G* methods, respectively. Full list of geometries parameters of PPy oligomers is summarized in Table S1 of the supplementary data section. From the results of RMSD, it can confirm the structural properties do not change significantly based on three methods. To avoid any misunderstanding, we have included the root mean square deviation formula in the revised manuscript.

Comment5 The sentence "The negative values of HOMO and LUMO can be used to estimate ionization potential and electron affinity, respectively." is wrong. What is the definition of ionization energy and electron affinity. In physics, ionization energy defines as the energy difference between vacuum level and Fermi level. Where is fermi level in your calculation? Of cause, it lies middle of HOMO and LUMO. Consequently, it has nothing to do with negative values of HOMO and LUMO.

Response: HOMO and LUMO can be directly used to estimate ionization potential and electron affinity. Please see the Paper>> Chang-Guo Zhan, Jeffrey A. Nichols, and David A. Dixon, Ionization Potential, Electron Affinity, Electronegativity, Hardness, and Electron Excitation Energy: Molecular Properties from Density Functional Theory Orbital Energies, J. Phys. Chem. A 2003, 107, 4184-4195. DOI: 10.1021/jp0225774. To reflect your concern, we have included a new reference in the revised manuscript. We hope that the revised version based on recommendations is now highly readable and solid for publication. Thanks again for your valuable time helping to improve this paper.