Review Form 1.6

Journal Name:	**Physical Science International Journal**
Manuscript Number:	**Ms_PSIJ_90692**
Title of the Manuscript:	**DENSITY FUNCTIONAL THEORY STUDY OF THE STRUCTURAL, ELECTRONIC, NON-LINEAR OPTICAL AND THERMODYNAMIC PROPERTIES OF POLY(3-HEXYLTHIOPHENE-2,5DIYL) IN GAS PHASE AND IN SOME SOLVENTS**
Type of the Article	**Original Research Article**

General guideline for Peer Review process:

This journal's peer review policy states that **NO** manuscript should be rejected only on the basis of '**lack of Novelty'**, provided the manuscript is scientifically robust and technically sound.
To know the complete guideline for Peer Review process, reviewers are requested to visit this link:

(https://www.journalpsij.com/index.php/PSIJ/editorial-policy)

PART 1: Review Comments

	Reviewer's comment	**Author's comment** *(if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)*
Compulsory REVISION comments		
Minor REVISION comments	1. Why do P3HT molecules have different bond lengths in different solvents? 2. The element represented by each atom in Figure 1 is unclear. It is recommended to refer to the representation in the paper (DOI: 10.1080/00387010.2011.607206). 3. It is recommended that the table and captions for Table 2 be kept on the same page. 4. Figure 2 is not clear. 5. The results of the IR spectra (**IR Intensities** section) are suggested to refer to these articles (DOI: 10.1016/j.saa.2011.06.008; 10.1007/s00396-004-1164-6). 6. Regarding the thermodynamic properties of the P3HT molecule based on theoretical calculations (**Thermodynamic Properties** section), it would be very helpful to suggest references to these papers (DOI: 10.1021/je300407g; 10.1016/j.jct.2016.06.009).	
Optional/General comments	**Comment**: This work reports the theoretical studies of P3HT in the gas phase and in certain solvents (methanol, thiophene, chloroform, toluene and acetone) based on DFT. The research results show that the frontier molecular orbital energy gap of P3HT molecules can be improved by choosing appropriate solvents and basis sets, which can be used for molecular device applications. This work is meaningful. However, revisions are required in the manuscript before publication.	

PART 2:

	Reviewer's comment	**Author's comment** *(if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)*
Are there ethical issues in this manuscript?	*(If yes, Kindly please write down the ethical issues here in details)*	

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