

Review Form 1.7

Journal Name:	Journal of Materials Science Research and Reviews
Manuscript Number:	Ms_JMSRR_95020
Title of the Manuscript:	Electronic Structure, Charge-transfer and Optical properties of Neutral, Anionic and Cationic Poly(3-hexylthiophene-2,5-diyl) (P3HT) Using DFT and TD-DFT Quantum Mechanical Methods
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://journaljmsrr.com/index.php/JMSRR/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 1. Is the manuscript important for scientific community? (Please write few sentences on this manuscript) 2. Is the title of the article suitable? (If not please suggest an alternative title) 3. Is the abstract of the article comprehensive? 4. Are subsections and structure of the manuscript appropriate? 5. Do you think the manuscript is scientifically correct? 6. Are the references sufficient and recent? If you have suggestion of additional references, please mention in the review form. (Apart from above mentioned 6 points, reviewers are free to provide additional suggestions/comments)	I think that this article is useful and it has some benefits for scientific community. I think that the title is extremely long and it should be shortened to "Using DFT and TD-DFT Quantum Mechanical Methods effects on Neutral, Anionic and Cationic Poly(3-hexylthiophene-2,5-diyl) (P3HT) Properties". The abstract of the article is comprehensive but long the others should focus on important results only. I think that the subsections and structure of the manuscript were appropriate in general. As far as I believe that this manuscript is scientifically appear to be correct. The references were sufficient and recent yet there were some references were very old [Ref. 2, 22 and 35]. No need for additional Ref. its already sufficient.	
Minor REVISION comments 1. Is language/English quality of the article suitable for scholarly communications?	The language is simple and plain English. Personally, I prefer that on pure English language. I believe that its more useful for foreign students.	
Optional/General comments	In general the article is fits the minimum scientific requirements.	

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?	<i>(If yes, Kindly please write down the ethical issues here in details)</i>	

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