



SDI Review Form 1.6

Journal Name:	Journal of Materials Science Research and Reviews
Manuscript Number:	Ms_JMSRR_45683
Title of the Manuscript:	Electronic Structure and Non-Linear Optical Properties of Neutral and Ionic Pyrene and its Derivatives based on Density Functional Theory
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:

(<http://www.sciencedomain.org/page.php?id=sdi-general-editorial-policy#Peer-Review-Guideline>)

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) For anionic and cationic species, an unpaired electron plays an important role. However, manuscript does not say anything about it and SOMO. Is it enough to discuss the properties of ionic species only considering HOMO and LUMO? (2) The basis set of 6-311G does not seem to be adequate for calculations of the anionic species. Therefore, discussion should be done on the results using the larger basis set. (3) p. 4, l. 8. $\epsilon_{\text{HOMO}} \rightarrow -\epsilon_{\text{HOMO}}$, $\epsilon_{\text{LUMO}} \rightarrow -\epsilon_{\text{LUMO}}$ (4) p. 4, Equation (7). $-(\epsilon_{\text{LUMO}} + \epsilon_{\text{HOMO}})/2 \rightarrow (\epsilon_{\text{LUMO}} + \epsilon_{\text{HOMO}})/2$ (5) p. 4, Equation (9). $\epsilon_{\text{LUMO}} - \epsilon_{\text{HOMO}}/2 \rightarrow (\epsilon_{\text{LUMO}} - \epsilon_{\text{HOMO}})/2$, $(\text{EA} - \text{IP})/2 \rightarrow (\text{IP} - \text{EA})/2$ (6) p. 6, ls 15-18. Duplication. (7) Tables 1 and 2 are meaningless without labels in figure. (8) Data are missing for anionic and cationic species at the B3LYP/6-311++G(d,p) level contrary to the description in the "Theoretical Methodology" section. (9) p. 7, l. 4. The comparison in the sentence "Addition of ... ionic forms." does not make sense. They are different bonds. (10) Please reconfirm the experimental value of R(C-Cl) for anionic and cationic species in Table 1. (11) Table 4 does not make sense. There are 4 to 7 energies for one species. (12) Please reconfirm the IP and EA values of anionic species in Table 5. Accordingly, discussion may be revised. (13) In conclusion. Please remove the last two sentences. No results in text.	1) Noted 2) 6-311+G(d,p) is included 3-11) correction were effected 12) The values were confirmed as they were before. 13) Done
Minor REVISION comments	(1) Please consider the number of significant figures in Tables and text. (2) Fig 2 $\rightarrow$ Fig 1, not cited. (3) Please unify the writing of the Table captions, "in neutral and charged state", "for neutral, anionic and cationic forms" or "for neutral and charged molecules."	1-3) Noted and corrected
Optional/General comments		



PART 2:

	Reviewer's comment	Author's comment <i>(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)</i>
Are there ethical issues in this manuscript?	<i>(If yes, Kindly please write down the ethical issues here in details)</i>	