



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	The analysis by Gaussiaon03 is well done. but some points are not cleared as mentioned below, 1) on page 4, the fundamental of DFT is much familiar, so please delà them 2) you changed standard basis set, 6-311G, 6-311+G(d), and 6-311++G(d,p). I am not sure what is the aime to change. 3) the relationship between gaussian03 and NOL proprettes is much weak. do you have some data of NOL and can you fit the calculation of molécules and experimental data? 4) Is there any idea to set the effective digit?	1) Noted but we don't think is a bad idea to give a brief of the theoretical background . 2) The basis sets were changed in order to see the effect of basis sets, its specification and the performance of each of the basis set under study on the properties. 3) No. 4) The values were reasonably compared to the pyrene family like pyrizine in the previous work.
Minor REVISION comments		
Optional/General comments		

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)	