



SDI Review Form 1.6

Journal Name:	Journal of Materials Science Research and Reviews
Manuscript Number:	Ms_JMSRR_50622
Title of the Manuscript:	Solvent Effects on the Structural, Electronic, Non-Linear Optical and Thermodynamic Properties of Perylene 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	<ol style="list-style-type: none"> 1. The content of the article should be concise and clear. When this increases and that decreases, what does it mean in conclusive sentences. There should also be a link and a summary of all these otherwise it can be very confusing. 2. Page 1. Line 7 should read "...applications such as organic photovoltaic cells, field effect transistors and biosensors." 3. Page 1. Line 13 should read "...package and revealed that..." 4. Page 1. Line 14 should read "...the bond lengths increase with..." 5. Page 1. Line 16 should read "Perylene molecule was found..." 6. Page 1. Line 20 should read "...and gas phase respectively,..." 7. Page 1. Line 22 should read "...in gas phase." 8. Page 1. Line 24 should read "...solvents. Similarly, the chemical..." 9. Page 1. Line 29. The polarity increases. So what? What's the point? 10. Page 1. Line 32. The polarity increases. So what? What's the point? 11. Page 1. Line 34 should read "...observed in chloroform due to..." 12. The common names of compounds are not necessary to be capitalized consistently all over the manuscript. 13. Page 1. Line 35 the energy gap is tuned. In what way? And it should read "...molecular orbital energy gap." 14. Page 2. Line 43 should read "...diodes, photovoltaic cells [1], organic..." 15. Page 2. Line 44 should read "...organic solar cells and transparent..." 16. Page 2. Line 46 should read "...information, their structural, electronic, optical, non-linear optical and thermodynamic properties are required." 17. Page 2. Line 48 should read "...general chemical formula C₁₀H_{4n+4} among which are the most widely investigated perylene (C₂₀H₁₂) and its derivatives such as perylenebisimides, (PTDCA) and.....(PDA) which, due to..." The full names of the compounds must be provided for the first time of mentioning them. 18. Page 2. Line 51 should read "...properties, are widely used..." 19. Page 2. Line 52 should read "...transistors, biolabels, sensors..." 20. Page 2. Line 54 should read "Interestingly, wide..." 21. Page 2. Line 55 should read "...applications of perylene and its derivatives including Density..." 22. Page 2. Line 56 should read "... (DFT) as well as a comparative..." 	



	<p>23. Page 2. Line 57 should read “Similarly, different exchange..”</p> <p>24. Page 2. Line 59 should read “..of perylene: insolated perylene,”</p> <p>25. Page 2. Line 60 should read “..lm]perylene (DIP) molecule and DIP molecular crystal were investigated [6]. The effect of...”</p> <p>26. Page 2. Line 62 should read “..forms (β-perylene), and...”</p> <p>27. Page 2. Line 63 should read “..forms (α-perylene) were studied [7]. The aggregation of...”</p> <p>28. Page 2. The third paragraph should say something about the results and the conclusive remarks obtained especially those concerning the topic under study, not just vaguely mention the reference.</p> <p>29. The standard form for referencing and stating the introduction is that the number of reference is put at the end and never use as a subject of sentences.</p> <p>30. Page 2. Line 66 should read “..in solution [2]. The structure and...”</p> <p>31. Page 2. Line 67 should read “..properties of pyrelene and coronene under pressure were also theoretically investigated using DFT [8] and Van der Waals interaction which were also used in obtaining the electronic structure of crystalline perylene [9]. However, to the best...”</p> <p>32. Page 3. Line 76 should read “..37.50) which were useful in.....” Conclusive remarks about the benefits from the investigation must be mentioned.</p> <p>33. Page 3. Line 84 should read “..a theory stating that all...”</p> <p>34. Page 3. Line 90. Why does the square need absolute value?</p> <p>35. Page 4. Line 114 should read “Unlike LDA and GGA, the hybrid function is a linear...”</p> <p>36. Page 4. Line 115 should read “..exchanges expressed as [14]:”</p> <p>37. Page 6. Line 141 should read “...perylene; the dipole...”</p> <p>38. Page 6. Line 154 should read “..by [16]:”</p> <p>39. Page 6. Line 156 should read “...defined as [16, 20]:”</p> <p>40. Page 6. Line 158 should read “...defined as:”</p> <p>41. Page 7. Line 168 should read “..used to evaluate...”</p> <p>42. Page 7. Line 175 should read “..geometry of perylene was...”</p> <p>43. Page 8. Line 203 should read “..isolated perylene molecule [6], the bond lengths here tend to be a little smaller. It is worth....”</p> <p>44. Page 8. Line 206 should read “..lengths of perylene in..”</p> <p>45. Page 8. Line 207 should read “..isolated perylene molecule.”</p> <p>46. Page 8. Line 209 should read “..of the optimized structure of perylene in the...”</p> <p>47. Page 9. Line 211 should read a[6]. The remark by author’s name and year is also acceptable, but this has to be consistent all aver the manuscript.</p> <p>48. Page 9. Line 212 should read “..of the optimized structure of perylene in the..”</p> <p>49. Page 9. Line 217 should read “However, the longest bond length..”. The greatest can also be used.</p> <p>50. Page 9. Line 219 should read “..in good agreement with those from previous work [6].”. But in [6] the compound is in the form of solid (crystal) so clearer discussion must be made on this basis of different states.</p> <p>51. Page 10. Line 221 should read “Table 3 presents the...”</p> <p>52. Page 10. Line 222 should read “..gaps of perylene in the...”</p> <p>53. Page 10. Line 235 should read “..energy of perylene in...”</p> <p>54. Page 10. Line 237 should read “....easier than that in the...”</p> <p>55. Page 10. Line 242 should read “..and energy gap of perylene in...”</p> <p>56. Page 11. Line 246 should read “Table 4 presents the...”</p> <p>57. Page 11. Line 249 should read “..from Table 4 that..”</p> <p>58. Page 12. Line 266 should read “..of the optimized structure of a perylene molecule..”</p> <p>59. Page 12. Line 277 should read “..in the gas phase with slightly higher value</p>	
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	<p>of..”</p> <p>60. Page 13. Line 284 should read “Table 7 presents..”</p> <p>61. Page 14. Line 302 should read “Table 8 presents..”. “Hence” here is not necessary and it does not make sense so it must be omitted.</p> <p>62. Page 14. Line 302 should read “..of perylene molecule..”</p> <p>63. Page 14. Line 310 should read “..Table 8 that perylene..”</p> <p>64. Page 14. Line 310 should read “..0.000eV both in the gas phase and in the solvents.”</p> <p>65. Page 14. Line 315 should read “..perylene.”</p> <p>66. Page 15. Line 321 should read “..presents the results of Natural...”</p> <p>67. Page 15. Line 322 should read “..of the optimized structure of perylene molecule..”</p> <p>68. Page 17. Line 327 should read “..Table 9 that the largest value..”</p> <p>69. Page 17. Line 328 should read “..of perylene was..”</p> <p>70. Page 17. Line 342 should read “..of perylene tend..”</p> <p>71. Page 17. Line 343 should read “..an isolated perylene as..”</p> <p>72. Page 17. Line 346 should read “..was found that the electron..”</p> <p>73. Page 18. Line 349 should read “..of perylene was..”</p> <p>74. Page 18. Line 351 should read “..of perylene increases..”</p> <p>75. Page 18. Line 358. Conclusive remark about future aspects should be implemented.</p> <p>76. Page 18. Line 367. Rev. no. May?!</p> <p>77. Page 19. Ref [10] and [13]. What are tehpages?</p> <p>78. Page 19. Ref [10] uses italic leteters whereas Ref [11] uses bold letters.</p> <p>79. Page 21. Ref [25] and [26]. What are the pages?</p> <p>80. Page 21. Line 438. Was it “Applied”?</p> <p>81. Page 21. Line 445 should read “Int. J. Techno. Chem. Res.”</p>	
<p>Minor REVISION comments</p>		
<p>Optional/General comments</p>		

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

Reviewer Details:

Name:	Pipat Chooto
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