



SDI Review Form 1.6

Journal Name:	Asian Journal of Chemical Sciences
Manuscript Number:	Ms_AJOCS_41530
Title of the Manuscript:	Quantum Investigation of Structure Electronic and Non-Linear Optical Properties of TTF Separated by Thiophene
Type of the 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		
Minor REVISION comments	1) The word "tetrathiafulvalene" have to be added in the abstract before TTF. 2) The introduction should be improved in terms of more background of the systems and the aim of the work. 3) Did the authors perform the frequency calculations to find that the systems are minima on the potential energy surface?. If not, the authors should run these calculations and complete the Material and methods section. 4) The first 3 lines in the MEP section (3.2) are not clear. Please correct the redaction. 5) The English has to be improved in the whole manuscript. 6) In Fig 3, please put the energy values of the orbitals in eV units. 7) How do the authors define A and IE? This information should be included. 8) The ionization potential is labelled as IE in table 5 but as I in the text. Please unify the data. 9) The Local Reactivity Descriptors section should be completed with clear information of how the authors got the indexes over the selected atoms and the criterium of the selection of the reported atoms in Table 6. Also, a better caption of Table 6 have to be included.	1) The word "tetrathiafulvalene" have been added in the abstract before TTF. 2) The introduction has been improved in terms background of the systems and the aim of the work (see introduction section) 3) The authors have performed the frequency calculations to find that the systems are minima on the potential energy surface (see Material and Methods and Molecular Geometry sections). 4) The first 3 lines in the MEP section have been corrected. 5) The English has been improved in the whole manuscript. 6) In Fig 3, the energy values of the orbitals have been converted on eV units. 7) A and IE have been defined and this information have been included. 8) The ionization potential is labelled as I and has been unified in the text. 9) The Local Reactivity Descriptors section has been completed with clear information. Also, a caption of Table 6 has been included.
Optional/General comments		