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Journal Name:	**Physical Science International Journal**
Manuscript Number:	**Ms_PSIJ_36555**
Title of the Manuscript:	**Structural and solvent dependence of the electronic properties and corrosion inhibitive potentials of 1,3,4-thiadiazole and its substituted derivatives- a theoretical investigation.**
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:

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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	**Physical Science International Journal** Manuscript Number: Ms_PSIJ_36555 Title: Structural and solvent dependence of the electronic properties and corrosion inhibitive potentials of 1,3,4-thiadiazole and its substituted derivatives- a theoretical investigation. Reply: The authors presented a frontier molecular orbital (FMO) investigation which is considered to be very important for describing chemical reactivity and understanding the the static molecular reactivity. The HOMO and LUMO orbital energies of 1,3,4 thiadiazole and its substituted derivatives were calculated using the hybrid B3LYP method with a large polar 6-31G* basis set in vacuum, acetone, ethanol and tetrahydrofuran (THF). It was revealed that substitution at position -2 with $-NO_2$, $-CH_3$, $-NH_2$, -CN and -CH=C(CN)COOH results in enhanced reactivities due to reduction of the energy gap, E_g. It is also altered some important molecular properties like η, S, ΔN, μ, α and β. Substituted $-NO_2$, -CN and -CH=C(CN)COOH may possess better inhibitive potentials and better reactivities than other derivatives on the basis of studied parameters. It was observed that solvent media affect molecular properties. The article is very well written and explains with clarity the main purpose of the investigation. Moreover, The results	

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	presented are good enough as to provide relevant chemical information that deserves to be accepted for publication at PSIJ.	
Minor REVISION comments	Accept it as it is.	
Optional/General comments	none	

Reviewer Details:

Name:	***Donald H. Galvan***
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