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Journal Name:	Physical Science International Journal
Manuscript Number:	**Ms_PSIJ_28273**
Title of the Manuscript:	**DFT Calculations of Mesembryanthemum nodiflorum compounds as Corrosion Inhibitors of Aluminum**
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	The work presented by the authors is based on theoretical (DFT) calculations. No experimental evidence is provided for any findings presented in the manuscript. Indeed, theoretical background is also needed to overcome some the unanswerable experimental findings. On this ground the manuscript is to be read and reviewed. My observation on the Manuscript- 1. As the authors have not isolated the species from the mixture it is likely that each and every functional group present in the molecule under consideration would likely to accelerate or inhibit the corrosion of Aluminum. In so what will be net effect and the interpretation of the theoretical calculation made? 2. HOMO and LUMO values are with the negative sign (Table 1). How the authors could state HOMO is of higher value than LUMO and also how to expect the transfer of electron from HOMO to LUMO? 3. Explanation/reason provided for the Data of Table 2 is not sufficient. It is difficult to understand why the calculations (LUMO inh – HOMO Al (eV) LUMO Al – HOMO inh (eV)) are made and in what way it helps in stating that inhibitor is of anodic or cathodic	

	type. What sort of inference can be drawn from LUMO inh – HOMO Al calculation? Method of evaluation of HOMO or LUMO is not available. Basis for the separation of different inhibitors into cathodic and anodic inhibitor is not available in the text. Can it be decided just by free energy value? 4. Method of evaluation of all the parameters of Table 3 is not known and moreover they have not been defined. Value of ΔN is too small and are almost equal (within the exptl.error?) to take any decision on the nature of bond present in the system (electrovalent or covalent), Electrophilicity value (ω) is the highest in case of Mesembren. It means it is a good acceptor of electron. Then how does the conclusion - Mesembren is a good inhibitor -arises? 5. Mesembrenone which has the lowest energy gap - Electron transfer is expected from HOMO of the species to LUMO of the metal. It is difficult to understand the authors decision that the largest inhibition efficiency is for the species Mesembrenone species? 6. All adsorption processes are spontaneous with a negative sign to ΔG . But on P.7 ΔG is shown with a positive sign. 7. P.6: Statement “Al atoms can accept electrons from inhibitor molecule to form a coordinated bond” (anodic inhibitor).How to support the statement?	

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	8. P 6:Explanation /mode of action for donation and back-donation processes strengthen the adsorption of Mesembrenone onto the aluminum surface and increase the inhibition efficiency is required Authors have given some theoretical foundation for the experimentalists to probe further before and either to approve or disapprove the fact. Theoretical materials scientists will really appreciate the content. However, the manuscript can be considered for publication as a note in the journal only after getting satisfactory explanation for above queries.	
Minor REVISION comments		
Optional/General comments		

Reviewer Details:

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