Review Form 3

Journal Name:	**Journal of Engineering Research and Reports**
Manuscript Number:	**Ms_JERR_130164**
Title of the Manuscript:	**Computational Study on Aluminum Corrosion Inhibitive Potentials of Preferred Thiosemicarbazide Derivatives**
Type of the Article	

PART 1: Comments

	Reviewer's comment	**Author's Feedback** *(Please correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)*
Please write a few sentences regarding the importance of this manuscript for the scientific community. A minimum of 3-4 sentences may be required for this part.	This article is highly relevant as it explores alternatives to traditional corrosion inhibitors, which pose significant risks to both human health and the environment. Many conventional inhibitors have been classified as carcinogenic, making the search for safer and more sustainable replacements essential.	
Is the title of the article suitable? (If not please suggest an alternative title)	Computational Analysis of Aluminum Corrosion Inhibition Using selected Thiosemicarbazide Derivatives	
Is the abstract of the article comprehensive? Do you suggest the addition (or deletion) of some points in this section? Please write your suggestions here.	Aluminum, a metal with a rich cultural history, remains vital in numerous industrial applications. However, its susceptibility to corrosion in harsh environments poses significant challenges. Traditional corrosion inhibitors have been developed to counteract this issue, but they often come with drawbacks such as high costs and harmful environmental and health impacts. This study employed density functional theory (DFT) to evaluate the potential of two compounds—2-(4-methylbenzylidene)hydrazinecarbothioamide (MBHC) and N-phenylhydrazinecarbothioamide (PHC)—as corrosion inhibitors for aluminum surfaces. Electrostatic potential (ESP) analysis revealed that the sulphur and nitrogen atoms in these compounds exhibit nucleophilic behaviour, making them effective for corrosion inhibition. The research highlighted MBHC's superior performance over PHC in corrosion prevention. Frontier molecular orbital theory and Monte Carlo simulations demonstrated that MBHC formed stronger and more stable complexes with the aluminum surface, as reflected in its higher adsorption energy of −461.73 eV compared to PHC's −163.43 eV. These findings pave the way for developing environmentally friendly inhibitors to protect aluminum surfaces, combining efficiency with sustainability.	
Is the manuscript scientifically, correct? Please write here.	Yes, the Manuscript is scientifically correct.	
Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.	The references are acceptable; however, it is recommended that references be more recent, preferably not older than four years.	

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Is the language/English quality of the article suitable for scholarly communications?	Yes.	
Optional/General comments	Manuscript is acceptable.	

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)*	

Reviewer Details:

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