Review Form 3

Journal Name:	**Asian Journal of Chemical Sciences**
Manuscript Number:	**Ms_AJOCS_124372**
Title of the Manuscript:	**First principle study of the adsorption of glyphosate on illite clay for water depollution.**
Type of the Article	**Original Research Article**

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PART 1: Review Comments

Compulsory REVISION 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. Why do you like (or dislike) this manuscript? A minimum of 3-4 sentences may be required for this part.	This manuscript is important for the scientific community because it addresses a pressing environmental and public health issue related to the contamination of groundwater with glyphosate residues, which are widely used in agriculture. By exploring the use of illite clay as an adsorbent for glyphosate through Density Functional Theory, it provides valuable insights into a potential solution for water purification. I appreciate the innovative approach of utilizing a natural and abundant material like illite, especially given its low environmental impact. However, I would have liked to see more experimental validation to complement the computational results, which could strengthen the practical application of the findings.	
Is the title of the article suitable? **(If not please suggest an alternative title)**	The title "First Principle Study of the Adsorption of Glyphosate on Illite Clay for Water Depollution" is suitable, as it clearly conveys the key focus of the research: using first-principles methods to study glyphosate adsorption on illite clay for water purification. However, for a more concise and impactful title, you might consider: **"First-Principles Investigation of Glyphosate Adsorption on Illite Clay for Water Purification"**	
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.	The abstract is generally comprehensive, covering the background, problem, methodology, and results. However, some aspects could be improved for clarity and focus. Here are a few suggestions: 1. **Clarify the Link to Health Outcomes**: The last sentence mentions the improvement in the management of cirrhotic patients, which seems disconnected from the rest of the abstract. If this is a significant part of the study, it should be explained earlier or better integrated. 2. **Remove or Refine Less Relevant Points**: The specific mention of "Benin" as a source of illite may not be essential in the abstract unless the location is directly related to the research objectives. 3. **Additional Suggestions**: o Highlight any comparison between illite and other materials if it was part of the study. o Mention the practical applications of the findings in water purification more explicitly.	
Are subsections and structure of the manuscript appropriate?	**yes**	
Please write a few sentences regarding the scientific correctness of this manuscript. Why do you think that this manuscript is scientifically robust and technically sound? A minimum of 3-4 sentences may be required for this part.	This manuscript appears to be scientifically robust and technically sound due to its use of Density Functional Theory (DFT) and the VASP simulation code, both of which are widely recognized as reliable computational tools for studying material interactions at the atomic level. The focus on adsorption properties and thermodynamics is well-grounded in established physical principles, ensuring that the theoretical framework is solid. The selection of illite clay, based on its abundance and non-toxic nature, demonstrates a clear understanding of practical and environmental concerns. However, the robustness of the manuscript could be further reinforced by including experimental validation to complement the theoretical findings.	
Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form. **-**	Look for recent publications on the use of various clays, especially illite, for environmental remediation. Include research published in the last 5 years that investigates glyphosate's environmental impact, particularly on groundwater and health risks. Cite the latest applications of Density Functional Theory and the VASP simulation code, particularly in environmental contexts. Include newer studies comparing the efficiency of illite to other materials (e.g., activated carbon, zeolites) for water purification.	

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Minor REVISION comments **Is the language/English quality of the article suitable for scholarly communications?**	The language of the article is generally understandable, but it could benefit from minor revisions to improve clarity, fluency, and readability. Example: "After use, its toxic residues and metabolites end up in groundwater, which is an important source of drinking water for the population." • Revised: "After use, toxic residues and metabolites from glyphosate enter groundwater, a critical source of drinking water." Example: "The absorbent properties, the abundance of illite throughout the world, particularly in Benin, and the fact that it is free from toxic products were the criteria that guide us in the of illite clay for our work." • Revised: "We selected illite clay for its abundant availability, non-toxic nature, and strong adsorbent properties, particularly in Benin."	
Optional/General comments	• Providing more context about the environmental and health implications of glyphosate contamination would help readers understand the significance of the study. Adding recent statistics or case studies could strengthen this section. • While the manuscript uses Density Functional Theory (DFT) and VASP simulation code, a brief overview of why these specific methods were chosen over others could be useful. Including a discussion on the limitations of the computational methods used might also add depth. • Suggesting specific areas for future research based on the study's findings would provide a helpful direction for subsequent studies. This could include exploring other types of adsorbents or investigating the long-term effects of using illite in water treatment. • Consider having the manuscript reviewed by a native English speaker or a professional editor to ensure that the language meets the highest standards of scholarly communication.	

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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