

Review Form 3

Journal Name:	Journal of Energy Research and Reviews
Manuscript Number:	Ms_JENRR_130790
Title of the Manuscript:	Numerical simulation and evaluation of Y2S3 and Y2TeS2 on structural, stability and electronic properties for photocatalytic water splitting applications
Type of the Article	Research

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PART 1: Comments

	Reviewer's comment	Author's Feedback <i>(Please correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)</i>
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.	Numerical simulation gives insights into complex interactions of photocatalytic materials used in the research. The Y2S3 and Y2TeS2 materials with promising structural properties studies in the manuscript may the best candidate for photo-conversion application and water splitting application	
Is the title of the article suitable? (If not please suggest an alternative title)	YES	
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.	YES	
Is the manuscript scientifically, correct? Please write here.	YES	
Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.	YES	
Is the language/English quality of the article suitable for scholarly communications?	Satisfactory.	
<u>Optional/General</u> comments	3. Results and Discussion 1) Calculated values of lattice parameters a,b,c for Y2S3, Y2TeS2 itself changing their change in %. The author are instructed to elaborate the discussion for why such change occurs due to addition of Te. 2) Authors are informed to explain how the value of poissons ratio from 0.1 to 0.25 linking/confirms to covalent bonding between Y2S3 and Y2TeS2 materials	Depending on the combination of the metal and chalcogenide (S, Se, and Te) elements, the physical properties such as structural, mechanical, dynamic, and electronic properties are modified \cite{Ref:36 – Ref:37}. The Poisson ratio describes the material nature of bonding characteristics, and material compressibility is related to shear modulus and Poisson's ratio. The ductility and brittleness of materials are distinguished based on Poisson's ratio, the material with a lower Poisson ratio exhibited a covalent nature of bonding because the directional nature of covalent bonding can limit lateral deformation. The Computed Poisson's ratio for Y\$\$_{2}S_{3}\$\$ and Y\$\$_{2}TeS_{2}\$\$, 0.24 and 0.25 respectively are seen in Table \ref{tbl:3}. The obtained values are lower suggesting that Y\$\$_{2}S_{3}\$\$ and Y\$\$_{2}TeS_{2}\$\$ are brittle materials, compressible, and can possess covalent or ionic bonding characteristics \cite{Ref:40}

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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)	