In the present work, the authors have proposed a data-driven high-throughput screening framework to identify high-performance single-atom catalysts (SACs) for hydrogen evolution and sensing applications. By integrating DFT calculations with graph neural networks (GNN), the authors systematically explore a wide materials space based on MXene-supported SACs. This work is timely, methodologically sound, and relevant to the materials and energy research community. The manuscript can be considered for publication after major revision.

1. The authors mention that "we expanded the dataset by processing crystal structure models intended for DFT calculations, increasing the original data volume fourfold" (Page 13). However, the procedure for this data augmentation is not clearly explained. The authors should elaborate on how the augmentation was performed and how it avoids introducing bias or overfitting in the machine learning model.
2. The manuscript does not address the thermal or chemical stability of the predicted SACs, which is crucial for real-world applications. While this may be outside the current scope, the authors should briefly comment on this limitation or suggest future validation strategies.
3. Ensure that the font size in all figure captions and axis labels is uniform and large enough to be clearly visible. Some plots (e.g., Figure 5) appear to have small, hard-to-read text.
4. The authors use the reaction energy $E[H_2]$ from the $H_2 + O \rightarrow H_2O$ process as a proxy for hydrogen sensing performance. However, this is not a conventional descriptor in gas sensor design literature. Most hydrogen sensing studies rely on adsorption energy, charge transfer, work function variation, or changes in conductivity upon H_2 exposure. The authors should justify the physical relevance of $E[H_2]$ in the context of sensing and provide literature references that support its use. A comparative discussion with standard descriptors would strengthen the methodology and help readers assess the generalizability of the results.

Overall, the present work is interesting and can be published after including these major comments.