The manuscript proposes valuable theoretical insights of the hydrogen absorption behaviour of high entropy alloys (TiZrHfScMo). Despite of all benefits the manuscript must be improved in order to be considered for publishing:

**Comment 1:** As proposed manuscript is based mostly on theoretical calculations it remains unclear why authors included information on alloy synthesis in "2. Computational details" and Fig.1 and Fig.3 in "3.1. The structural parameters....".
Response: The aim of this study is to evaluate the potential of TiZrHfScMo high entropy alloy (HEA) as a hydrogen storage material by density functional theory calculations. This new material has not been synthesized and reported in the literature thus far. Thus, we synthesized the TiZrHfScMo HEA and characterized its structure by in situ XRD. The experimental results in this study proves that the new TiZrHfScMo HEA can be synthesized and its structure is BCC phase.
In the revised manuscript, the title of section 2 has been modified as “Computational and experimental details”.

**Comment 2:** Fig. 1 presents the XRD of the alloy as obtained. What is the added value of this XRD results? If it could be kept would be useful to add XRD results after alloy hydrogenation too.
Response: Please see the response to comment 1.

**Comment 3:** I would suggest to extend all experimental activities in separate publication and present all experimental results in details.
Response: Thanks for the reviewer’s suggestions. Yes, experimental investigation of the hydrogen storage stability will be carried out in the future work and another publication will present all the experimental results in details.

**Comment 4:** Both of Fig.1. and Fig. 3 could be excluded or authors need to rewrite Abstract and Conclusions where these experimental activities and results not mentioned.
Response: In the revised manuscript, the abstract and conclusions have been rewritten.