In the work with title "A DFT study of hydrogen storage in high entropy alloy TiZrHfScMo" a theoretical study on the behaviour of TiZrHfScMo alloy in the hydrogen adsorption is carried out. DFT calculations are very attractive and powerful tool and any work in this field is welcome. The present work can be accepted with some minor modifications. Following, there are some required clarifications:

**Comment 1:** Is the TiZrHfScMo alloy actually synthesised? How?
Response: Yes, the equiatomic Ti, Zr, Hf, Sc and Mo metals are weighed to synthesize the TiZrHfScMo alloy by the arc-melting method. All of the raw materials are in the shape of small particles between 1 and 10 mm and have a purity of 99.99%. The alloy ingot is re-melted five times to improve the homogeneity of each element. The details have been described on page 3, lines 89-95.

**Comment 2:** Regarding to X-ray diffraction authors reported the lattice constant but not any other parameter such as particle size?
Response: The particle size is 104.2±52.3 um, which has been described on page 3, line 92.

**Comment 3:** Why is important to determine the lattice constant?
Response: The TiZrHfScMo alloy in this study is a new high-entropy alloy, for which the structural phase and lattice constant has not been reported thus far and the related information are not available in the literature. In our DFT calculation, the structural phase is necessary for the building of structural model and the lattice constant is necessary to test the validity of our calculations. Hence, the lattice constant is an important parameter.

**Comment 4:** In figure 2 is quite difficult to appreciate differences, apart from the increasing number of hydrogen atoms. Is there any other noticeable difference?
Response: With the increasing number of hydrogen atoms, the displacement of alloy elements is more significant. This is caused by the interaction between hydrogen atoms and metal atoms.