

Contribution ID : **239** Type : **Poster**

Interstitial Hydrogen Trapping in TiVZrNbHf High-Entropy Alloy: DFT-Based Training and Predictive Evaluation of MACE Potential

High-entropy alloys (HEAs) have attracted considerable interest as potential hydrogen storage materials due to the diversity of their local chemical environments and interstitial sites. In particular, the equiatomic TiVZrNbHf alloy, with a body-centered cubic (BCC) structure, exhibits a high hydrogen absorption capacity, associated with lattice distortions and the presence of different interstitial sites [1, 2]. This work investigates interstitial hydrogen stability in TiVZrNbHf using a methodology that combines density functional theory (DFT) calculations and MACE machine learning interatomic potentials. Five special quasirandom structures (SQS) are considered to represent the chemical disorder of the alloy. Within these structures, interstitial hydrogen configurations, including octahedral, tetrahedral, and randomly selected sites, are evaluated to explore the influence of local atomic environments on their stability. DFT results are used to fine-tune the pre-trained MACE-MP-0 model. Its predictive capability is assessed through an intra-configuration generalization strategy, in which the training, validation, and test sets contain distinct interstitial sites belonging to the same five SQS configurations. The energies and atomic forces predicted by MACE are compared with DFT reference values to determine its ability to reproduce previously unseen interstitial environments within known chemical configurations and to identify potentially favorable sites for hydrogen trapping.

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Session Classification : Poster Fisica del Estado Solido