Ab initio simulations of Laves-phase high-entropy alloys for hydrogen storage

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High-entropy alloys (HEAs), particularly those in the Laves phases, are promising candidates for hydrogen-storage alloys. Recent experiments have indeed revealed that the equiatomic TiZrCrMnFeNi Laves-phase HEA can work as a hydrogen-storage alloy at room temperature (i.e., without heating) under nearly atmospheric pressure [1,2]. Tuning the compositions of such Laves-phase HEAs should be possible to design hydrogen-storage alloys with more desirable properties. We have demonstrated that *ab initio* H adsorption energies in $Ti_xZr_{2-x}CrMnFeNi$ become more negative (thus energetically more favorable) on average with increasing the Ti content, consistent with experiments [3]. We will also show how the H adsorption energy depends on the local chemical environment in the Laves-phase HEAs.

References

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