

Supplementary material for

First-principles investigation of alloying element effects on Hydrogen trapping and diffusion at the α -Fe/VC interface and within the VC bulk

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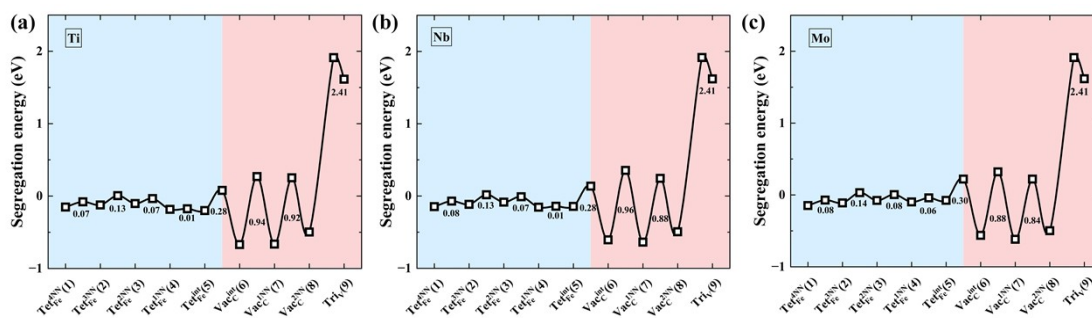


Fig. S1 Diffusion pathways and corresponding energy barriers for a H atom migrating from the Fe side into the VC side. Energy barriers in the interface doped with (a) Ti, (b) Nb, and (c) Mo.

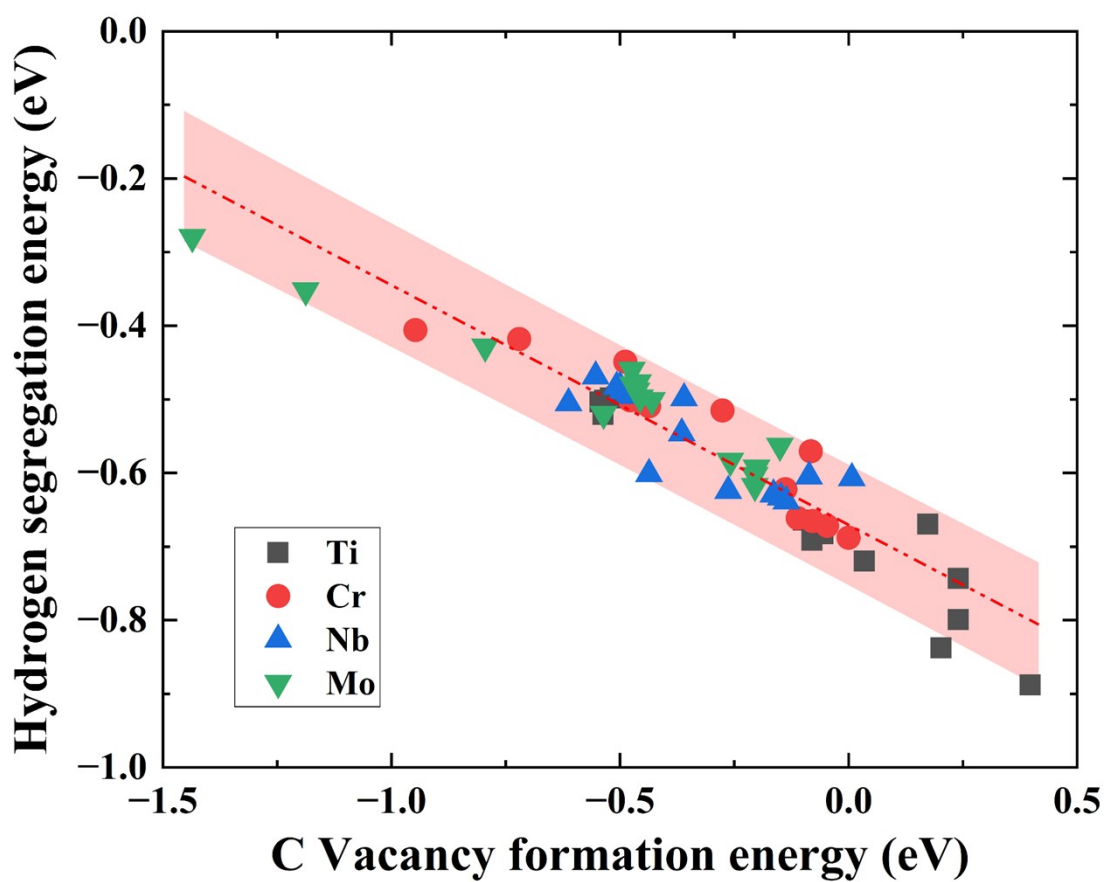


Fig. S2 The relationship between C vacancy formation energy and hydrogen segregation energy.