

Revealing the effect of NbH_x(x=1,2)/MgH₂ interface on MgH₂ dehydrogenation from first-principles

Yukun Liu, Jianchuan Wang*, Changbin Wei, Linkun Zhang, Bo Han, Yong Du

State Key Laboratory of Powder Metallurgy, Central South University, Changsha 410083, China

Corresponding authors. E-mail addresses: jcwang@csu.edu.cn

Table S1. The calculated lattice parameters for bulk MgH₂ and NbH₂

	MgH ₂		NbH ₂	Nb
	a(Å)	c(Å)	a(Å)	a(Å)
This work	4.501	3.013	4.557	3.312
Other DFT	4.487 ^[1]	2.994 ^[1]	4.580 ^[2]	3.321 ^[2]
Exp.	4.501 ^[3]	3.010 ^[3]	4.562 ^[4]	3.299 ^[4]

Table S2. Surface energy of NbH₂(100), NbH₂(110), and NbH₂(111) slabs

Surface	NbH ₂ (100)	NbH ₂ (110)	NbH ₂ (111)
Surface energy (eV/Å ²)	2.49	2.13	2.93

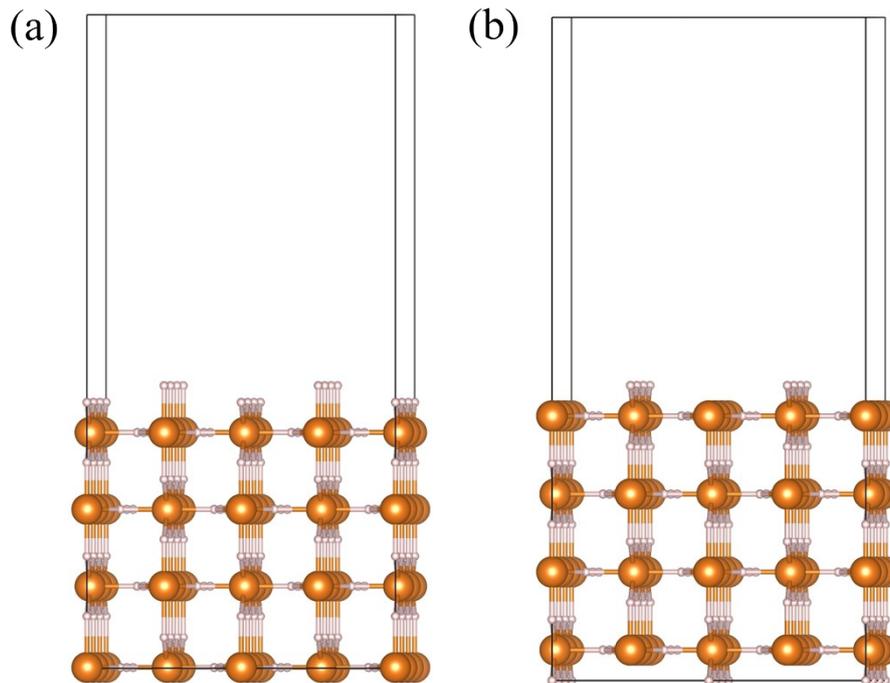


Fig. S1. The atomic structure of (a) H1-terminated and (b) H2-terminated MgH₂(110) slab. The orange and pink balls represent Mg and H atoms, respectively.

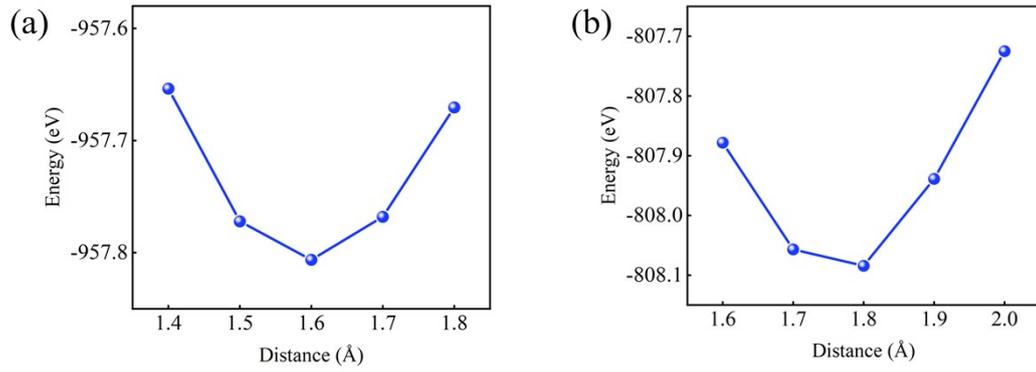


Fig. S2. Surface distance test of (a) NbH₂(110)/MgH₂(110) interface, (b) NbH(110)/MgH₂(110) interface.

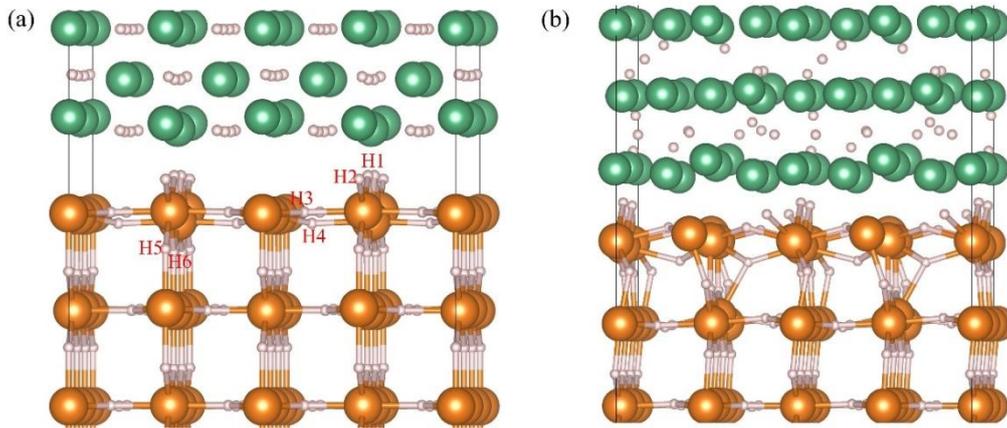


Fig. S3. The relaxed interface of (a) NbH₂(110)/MgH₂(110) interface, and (b) NbH(110)/MgH₂(110) interface. H1-H6 are the six hydrogen atoms in different coordination environments in the first three layers of NbH₂(110)/MgH₂(110) interface.

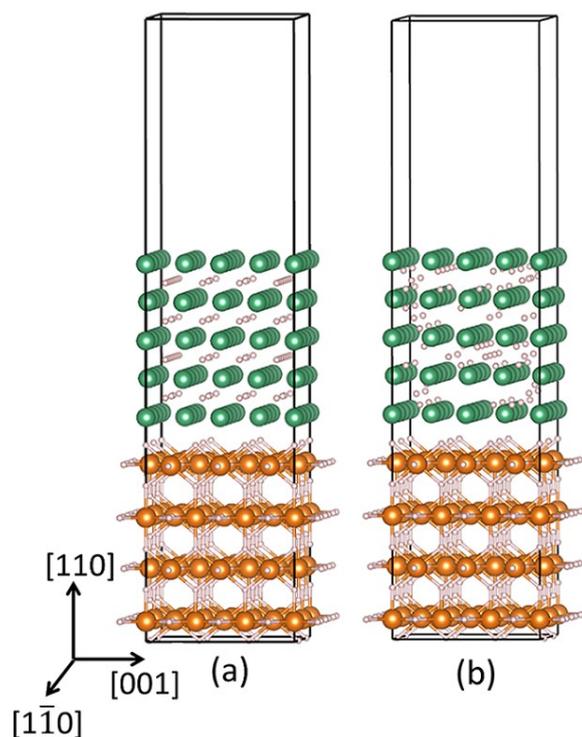


Fig. S4. Atomic structure of (a) ordered NbH(110)/MgH₂(110) interface and (b) disordered NbH(110)/MgH₂(110) interface #2. The orange, pink, and green spheres represent Mg, H, and Nb atoms, respectively.

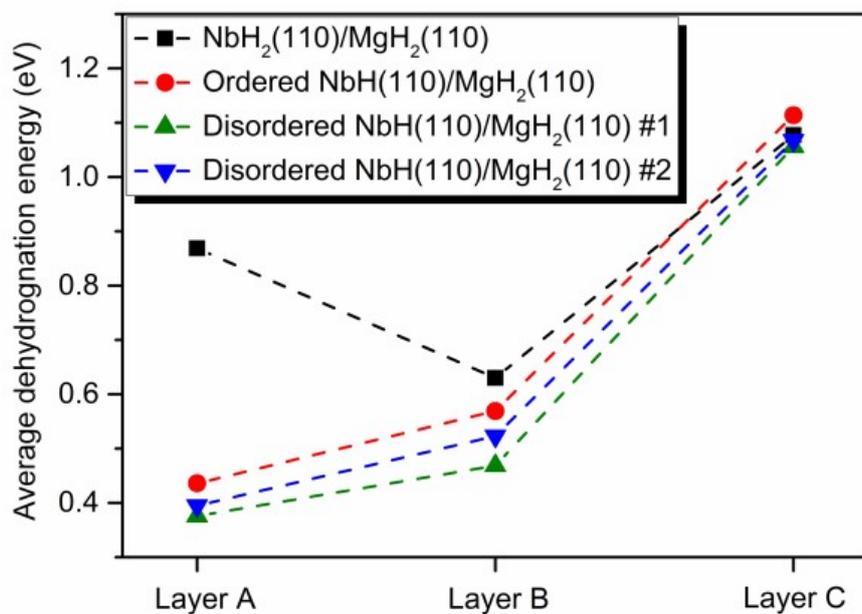


Fig. S5. The average dehydrogenation energies of Layer A, Layer B and Layer C.

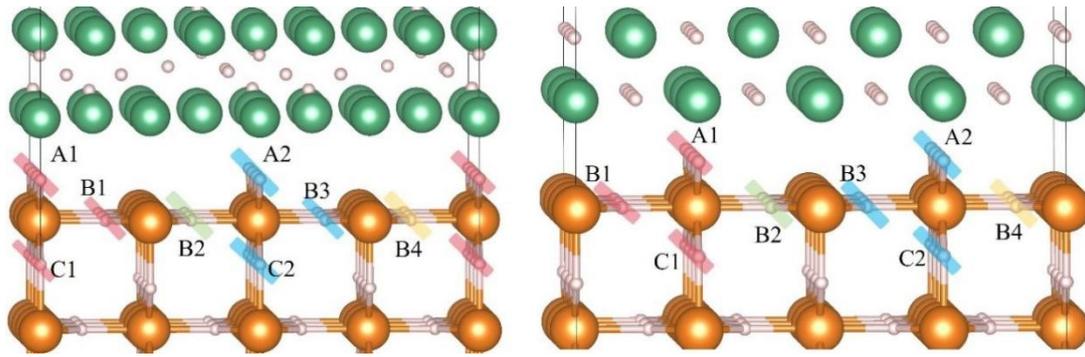
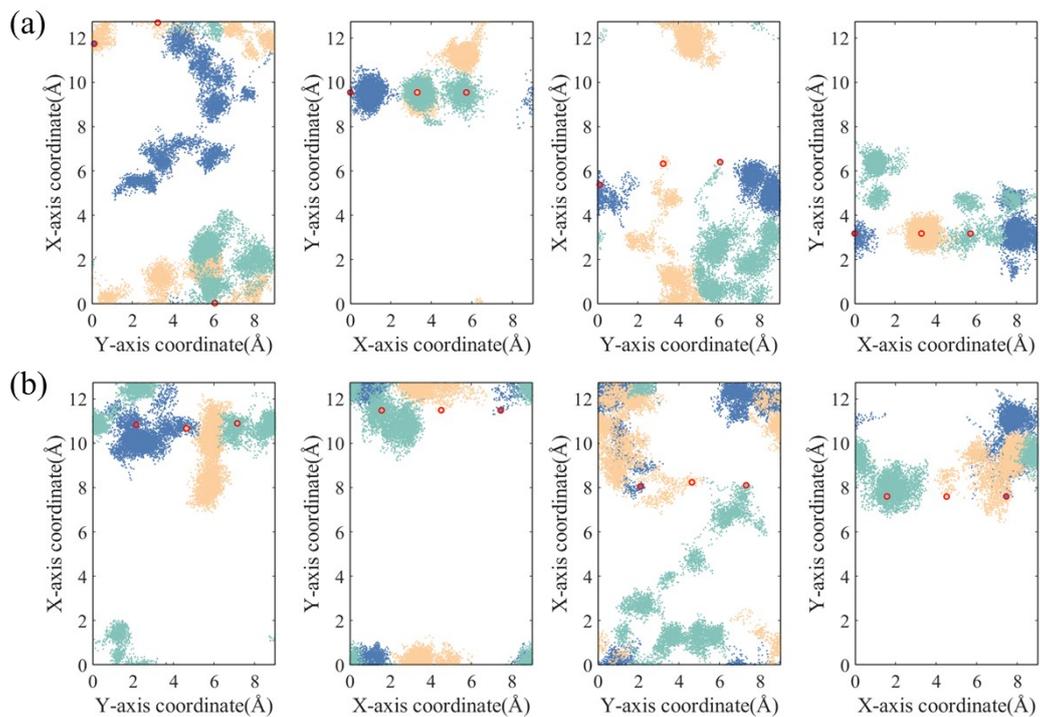


Fig. S6. Atomic diagrams of A1, A2, B1, B2, B3, B4, C1, C2. At the interface layer (layer A), the red and blue parts of hydrogen atoms are A1 and A2. At the sub-interface layer (layer B), red, b-interface green, blue and yellow parts of hydrogen atoms are B1, B2, B3 and B4, respectively. At the lower-sub-interface layer (layer C), the red and blue parts of hydrogen atoms are C1 and C2.



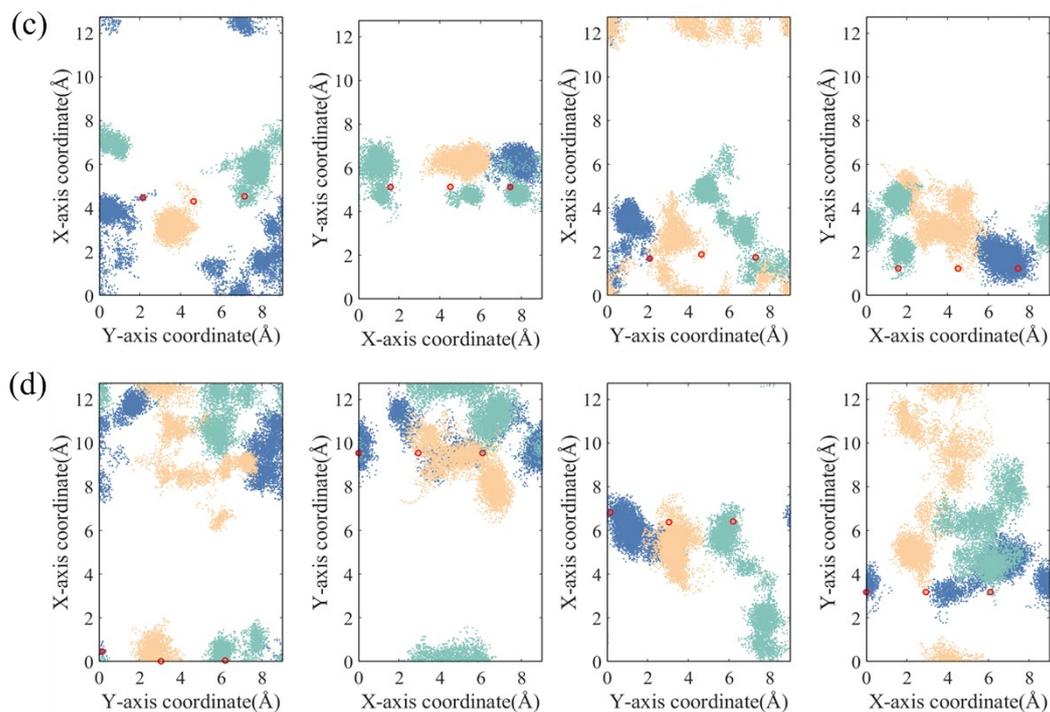


Fig. S7. Two-dimensional trajectories of the three layers of H atoms in the interface. (a) represent H atoms of A1 and A2, (b) represent H atoms of B1 and B2, (c) represent H atoms of B3 and B4, (d) represent H atoms of C1 and C2. The horizontal coordinate is X-axis for $\text{NbH}_2(110)/\text{MgH}_2(110)$ interface and Y-axis for $\text{NbH}(110)/\text{MgH}_2(110)$. The red dots are the initial positions of H atoms.

References

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