

Supplementary Information

MgH₂/Single-Atom Heterojunctions: Effective Hydrogen Storage Materials with Facile Dehydrogenation

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Table S1. The distance-energy relationship between MgH₂ and SAC-Ni.

Distance (Å)	Energy (eV)
2.0	-802.7053487
2.5	-806.0292115
3.0	-806.3217833
3.5	-806.1569593
4.0	-806.1008051
4.5	-805.6427083
5.0	-805.5830351

Table S2. Summary of DFT calculated energies (E_{DFT}), entropy changes (ΔTS), zero-point energies (E_{ZPE}), and Gibbs free energies (G) of the initial states (IS) of MgH₂/SACs-TM (TM = Ti, V, Cr, Mn, Fe, Co, Ni, Cu, and Zn).

Structure	E_{DFT} (eV)	ΔTS (eV)	E_{ZPE} (eV)	G (eV)
MgH ₂	-273.6836	0.0080	0.5992	-273.0925
MgH ₂ @Ti	-809.4451	0.1019	2.1034	-807.4437
MgH ₂ @V	-809.5338	0.1121	1.6713	-807.9746
MgH ₂ @Cr	-808.9755	0.0785	2.1335	-806.9206
MgH ₂ @Mn	-810.0540	0.1045	2.1872	-807.9713
MgH ₂ @Fe	-809.0279	0.1001	2.0445	-807.0835
MgH ₂ @Co	-808.1046	0.0817	2.1569	-806.0294
MgH ₂ @Ni	-808.2033	0.1168	1.5503	-806.7698
MgH ₂ @Cu	-803.9752	0.1172	1.6670	-802.4254
MgH ₂ @Zn	-801.4759	0.0938	2.1158	-799.4539

Table S3. Summary of DFT calculated energies (E_{DFT}), entropy changes (ΔTS), zero-point energies (E_{ZPE}), and Gibbs free energies (G) of the transition states (TS) of MgH₂/SACs-TM (TM = Ti, V, Cr, Mn, Fe, Co, Ni, Cu, and Zn).

Structure	E_{DFT} (eV)	ΔTS (eV)	E_{ZPE} (eV)	G (eV)
MgH ₂	-270.4298	0.0065	0.7867	-269.6497
MgH ₂ @Ti	-808.1631	0.0890	2.0384	-806.2138
MgH ₂ @V	-808.1207	0.1044	1.9643	-806.2609
MgH ₂ @Cr	-807.3113	0.0787	2.1252	-805.2648
MgH ₂ @Mn	-808.0372	0.0925	1.9263	-806.2034
MgH ₂ @Fe	-807.6766	0.1156	2.0300	-805.7622
MgH ₂ @Co	-805.6578	0.0952	1.9631	-803.7898
MgH ₂ @Ni	-805.5945	0.0728	1.8680	-803.7993
MgH ₂ @Cu	-801.4995	0.1085	1.8815	-799.7265
MgH ₂ @Zn	-799.0528	0.0966	2.2892	-796.8602

Table S4. Summary of DFT calculated energies (E_{DFT}), entropy changes (ΔTS), zero-point energies (E_{ZPE}), and Gibbs free energies (G) of the final states (FS) of $MgH_2/SACs-TM$ (TM = Ti, V, Cr, Mn, Fe, Co, Ni, Cu, and Zn).

Structure	E_{DFT} (eV)	ΔTS (eV)	E_{ZPE} (eV)	G (eV)
MgH_2	-271.3904	0.0051	1.0846	-270.3109
$MgH_2@Ti$	-808.4936	0.1220	2.0842	-806.5315
$MgH_2@V$	-808.1310	0.1286	1.8124	-806.4471
$MgH_2@Cr$	-807.4452	0.0859	2.1675	-805.3635
$MgH_2@Mn$	-808.0352	0.1175	1.8322	-806.3205
$MgH_2@Fe$	-807.9092	0.1482	1.6170	-806.4403
$MgH_2@Co$	-806.0228	0.0901	1.8824	-804.2306
$MgH_2@Ni$	-805.9854	0.0945	1.6918	-804.3882
$MgH_2@Cu$	-802.2433	0.1173	1.7956	-800.5650
$MgH_2@Zn$	-799.0419	0.1240	1.7355	-797.4304

Table S5. Predicted dehydrogenation temperature for MgH₂/SACs assuming MgH₂ dehydrogenation at 700 K.

Materials	E_a (eV)	T (K)
MgH ₂	3.44	700
MgH ₂ /SAC-Ti	1.217	247.65
MgH ₂ /SAC-V	1.706	347.15
MgH ₂ /SAC-Cr	1.656	336.96
MgH ₂ /SAC-Mn	1.756	357.30
MgH ₂ /SAC-Fe	1.337	272.02
MgH ₂ /SAC-Co	2.253	458.47
MgH ₂ /SAC-Ni	2.927	595.53
MgH ₂ /SAC-Cu	2.690	547.42
MgH ₂ /SAC-Zn	2.596	528.35

Table S6. Comparison of the dehydrogenation performance of MgH₂/SAC-TM with those of previous materials. The statistics contain the pure MgH₂ dehydrogenation energy barrier (E_d), and the percentage reduction of the dehydrogenation energy barrier (R_a).

Materials	E_d (eV)	R_a	Functional
MgH ₂ /SAC-Ti	1.217	0.646	GGA_PBE
MgH ₂ /TM(3d)	0.476	0.222	GGA_PW91
MgH ₂ /LiAl	1.956	0.309	GGA_PW91
MgH ₂ /BPG	1.050	0.557	GGA_PBE

Table S7. -IPCOHP of each orbital between the two atoms corresponding to Bond 1 of MgH₂ in **Figure 7**.

AtomMU	AtomNU	Distance (Å)	-IPCOHP (arb. units)
H74	Mg18	1.85273	0.98432
H74_1s	Mg18_3s	1.85273	0.94311
H74_1s	Mg18_2p_y	1.85273	0.00006
H74_1s	Mg18_2p_z	1.85273	0.00341
H74_1s	Mg18_2p_x	1.85273	0.03776
H74_1s	Mg18_2p_total	1.85273	0.04122

Table S8. -IPCOHP of each orbital between the two atoms corresponding to Bond 2 of MgH₂ in **Figure 7**.

AtomMU	AtomNU	Distance (Å)	-IPCOHP (arb. units)
H74	Mg22	1.85273	0.99282
H74_1s	Mg22_3s	1.85273	0.94249
H74_1s	Mg22_2p_y	1.85273	0.00003
H74_1s	Mg22_2p_z	1.85273	0.00323
H74_1s	Mg22_2p_x	1.85273	0.04708
H74_1s	Mg22_2p_total	1.85273	0.05034

Table S9. -IPCOHP of each orbital between the two atoms corresponding to Bond 1 of MgH₂/SACs-Ti in **Figure 7**.

AtomMU	AtomNU	Distance (Å)	-IPCOHP (arb. units)
H90	Mg26	2.11946	0.36083
H90_1s	Mg26_3s	2.11946	0.32765
H90_1s	Mg26_2p_y	2.11946	-0.00013
H90_1s	Mg26_2p_z	2.11946	0.00002
H90_1s	Mg26_2p_x	2.11946	0.03329
H90_1s	Mg26_2p_total	2.11946	0.03318

Table S10. -IPCOHP of each orbital between the two atoms corresponding to Bond 2 of MgH₂/SACs-Ti in **Figure 7**.

AtomMU	AtomNU	Distance (Å)	-IPCOHP (arb. units)
H90	Mg30	2.11946	0.54170
H90_1s	Mg30_3s	2.11946	0.51679
H90_1s	Mg30_2p_y	2.11946	0.00057
H90_1s	Mg30_2p_z	2.11946	0.01095
H90_1s	Mg30_2p_x	2.11946	0.01340
H90_1s	Mg30_2p_total	2.11946	0.02492

Table S11. -IPCOHP of each orbital between the five atoms of MgH₂/SACs-Co in **Figure 7** and **Figure S6**.

AtomMU	AtomNU	Distance (Å)	-IPCOHP (arb. units)
H90	Mg26	1.89576	0.91543
H90_1s	Mg26_3s	1.89576	0.86164
H90_1s	Mg26_2p_y	1.89576	0.00006
H90_1s	Mg26_2p_z	1.89576	0.00725
H90_1s	Mg26_2p_x	1.89576	0.04649
H90	Mg30	1.87044	0.95071
H90_1s	Mg30_3s	1.87044	0.89721
H90_1s	Mg30_2p_y	1.87044	-0.00003
H90_1s	Mg30_2p_z	1.87044	0.00693
H90_1s	Mg30_2p_x	1.87044	0.04661
Mg18	H66	1.88152	0.97221
Mg18_3s	H66_1s	1.88152	0.92325
Mg18_2p_y	H66_1s	1.88152	0.00001
Mg18_2p_z	H66_1s	1.88152	0.00471
Mg18_2p_x	H66_1s	1.88152	0.04424
H66	Mg30	1.88486	0.93484
H66_1s	Mg30_3s	1.88486	0.89179
H66_1s	Mg30_2p_y	1.88486	0.00014
H66_1s	Mg30_2p_z	1.88486	0.00349

H66_1s	Mg30_2p_x	1.88486	0.03941
Mg18	H74	1.86457	0.91447
Mg18_3s	H74_1s	1.86457	0.88160
Mg18_2p_y	H74_1s	1.86457	-0.00002
Mg18_2p_z	H74_1s	1.86457	0.00208
Mg18_2p_x	H74_1s	1.86457	0.03080

Table S12. -IPCOHP of each orbital between the five atoms of MgH₂/SACs-Cr in **Figure 7** and **Figure S6**.

AtomMU	AtomNU	Distance (Å)	-IPCOHP (arb. units)
H90	Mg26	1.98252	0.75102
H90_1s	Mg26_3s	1.98252	0.68779
H90_1s	Mg26_2p_y	1.98252	0.00019
H90_1s	Mg26_2p_z	1.98252	0.01694
H90_1s	Mg26_2p_x	1.98252	0.04611
H90	Mg30	1.91713	0.8419
H90_1s	Mg30_3s	1.91713	0.78068
H90_1s	Mg30_2p_y	1.91713	0.00035
H90_1s	Mg30_2p_z	1.91713	0.01447
H90_1s	Mg30_2p_x	1.91713	0.04641
Mg18	H66	1.88306	0.95766
Mg18_3s	H66_1s	1.88306	0.90011
Mg18_2p_y	H66_1s	1.88306	0.00006
Mg18_2p_z	H66_1s	1.88306	0.00761
Mg18_2p_x	H66_1s	1.88306	0.04988
H66	Mg30	1.85893	0.97086
H66_1s	Mg30_3s	1.85893	0.90585
H66_1s	Mg30_2p_y	1.85893	0.00003
H66_1s	Mg30_2p_z	1.85893	0.01039

H66_1s	Mg30_2p_x	1.85893	0.0546
Mg18	H74	1.87924	0.92477
Mg18_3s	H74_1s	1.87924	0.88496
Mg18_2p_y	H74_1s	1.87924	0.00005
Mg18_2p_z	H74_1s	1.87924	0.00534
Mg18_2p_x	H74_1s	1.87924	0.03442

Table S13. -IPCOHP of each orbital between the five atoms of MgH₂/SACs-Cu in **Figure 7** and **Figure S6**.

AtomMU	AtomNU	Distance (Å)	-IPCOHP (arb. units)
H90	Mg26	1.91349	0.91099
H90_1s	Mg26_3s	1.91349	0.85047
H90_1s	Mg26_2p_y	1.91349	0.00008
H90_1s	Mg26_2p_z	1.91349	0.00916
H90_1s	Mg26_2p_x	1.91349	0.05128
H90	Mg30	1.88233	0.94549
H90_1s	Mg30_3s	1.88233	0.89284
H90_1s	Mg30_2p_y	1.88233	0.00016
H90_1s	Mg30_2p_z	1.88233	0.00684
H90_1s	Mg30_2p_x	1.88233	0.04565
Mg18	H66	1.88152	0.96724
Mg18_3s	H66_1s	1.88152	0.91785
Mg18_2p_y	H66_1s	1.88152	0.00002
Mg18_2p_z	H66_1s	1.88152	0.00408
Mg18_2p_x	H66_1s	1.88152	0.0453
H66	Mg30	1.88486	0.93866
H66_1s	Mg30_3s	1.88486	0.89208
H66_1s	Mg30_2p_y	1.88486	0.00016
H66_1s	Mg30_2p_z	1.88486	0.00506

H66_1s	Mg30_2p_x	1.88486	0.04137
Mg18	H74	1.86457	0.90924
Mg18_3s	H74_1s	1.86457	0.87852
Mg18_2p_y	H74_1s	1.86457	-0.00001
Mg18_2p_z	H74_1s	1.86457	0.00221
Mg18_2p_x	H74_1s	1.86457	0.02852

Table S14. -IPCOHP of each orbital between the five atoms of MgH₂/SACs-Ni in **Figure 7** and **Figure S6**.

AtomMU	AtomNU	Distance (Å)	-IPCOHP (arb. units)
H90	Mg26	1.88623	0.95294
H90_1s	Mg26_3s	1.88623	0.89448
H90_1s	Mg26_2p_y	1.88623	-0.00002
H90_1s	Mg26_2p_z	1.88623	0.00629
H90_1s	Mg26_2p_x	1.88623	0.0522
H90	Mg30	1.88196	0.95238
H90_1s	Mg30_3s	1.88196	0.90323
H90_1s	Mg30_2p_y	1.88196	0.00001
H90_1s	Mg30_2p_z	1.88196	0.00734
H90_1s	Mg30_2p_x	1.88196	0.0418
Mg18	H66	1.88772	0.98409
Mg18_3s	H66_1s	1.88772	0.94057
Mg18_2p_y	H66_1s	1.88772	0.00004
Mg18_2p_z	H66_1s	1.88772	0.00429
Mg18_2p_x	H66_1s	1.88772	0.03919
H66	Mg30	1.88081	0.9659
H66_1s	Mg30_3s	1.88081	0.92314
H66_1s	Mg30_2p_y	1.88081	0.00006
H66_1s	Mg30_2p_z	1.88081	0.00403

H66_1s	Mg30_2p_x	1.88081	0.03867
Mg18	H74	1.85983	0.94382
Mg18_3s	H74_1s	1.85983	0.89578
Mg18_2p_y	H74_1s	1.85983	0.00015
Mg18_2p_z	H74_1s	1.85983	0.00272
Mg18_2p_x	H74_1s	1.85983	0.04516

Table S15. -IPCOHP of each orbital between the five atoms of MgH₂/SACs-V in **Figure 7** and **Figure S6**.

AtomMU	AtomNU	Distance (Å)	-IPCOHP (arb. units)
H90	Mg26	2.00803	0.71316
H90_1s	Mg26_3s	2.00803	0.64764
H90_1s	Mg26_2p_y	2.00803	0.00033
H90_1s	Mg26_2p_z	2.00803	0.01802
H90_1s	Mg26_2p_x	2.00803	0.04717
H90	Mg30	1.97744	0.74448
H90_1s	Mg30_3s	1.97744	0.68251
H90_1s	Mg30_2p_y	1.97744	0.00007
H90_1s	Mg30_2p_z	1.97744	0.01623
H90_1s	Mg30_2p_x	1.97744	0.04567
Mg18	H66	1.88152	0.96254
Mg18_3s	H66_1s	1.88152	0.90876
Mg18_2p_y	H66_1s	1.88152	0.00001
Mg18_2p_z	H66_1s	1.88152	0.00625
Mg18_2p_x	H66_1s	1.88152	0.04752
H66	Mg30	1.88486	0.95141
H66_1s	Mg30_3s	1.88486	0.87199
H66_1s	Mg30_2p_y	1.88486	0.00014
H66_1s	Mg30_2p_z	1.88486	0.0121

H66_1s	Mg30_2p_x	1.88486	0.06718
Mg18	H74	1.86457	0.92499
Mg18_3s	H74_1s	1.86457	0.89153
Mg18_2p_y	H74_1s	1.86457	-0.00002
Mg18_2p_z	H74_1s	1.86457	0.00243
Mg18_2p_x	H74_1s	1.86457	0.03106

Table S16. -IPCOHP of each orbital between the five atoms of MgH₂/SACs-Zn in **Figure 7** and **Figure S6**.

AtomMU	AtomNU	Distance (Å)	-IPCOHP (arb. units)
H90	Mg26	1.89576	0.93658
H90_1s	Mg26_3s	1.89576	0.87985
H90_1s	Mg26_2p_y	1.89576	0.00007
H90_1s	Mg26_2p_z	1.89576	0.00885
H90_1s	Mg26_2p_x	1.89576	0.04781
H90	Mg30	1.87044	0.96858
H90_1s	Mg30_3s	1.87044	0.9144
H90_1s	Mg30_2p_y	1.87044	0
H90_1s	Mg30_2p_z	1.87044	0.00791
H90_1s	Mg30_2p_x	1.87044	0.04627
Mg18	H66	1.88152	0.97432
Mg18_3s	H66_1s	1.88152	0.9247
Mg18_2p_y	H66_1s	1.88152	0.00004
Mg18_2p_z	H66_1s	1.88152	0.00439
Mg18_2p_x	H66_1s	1.88152	0.04518
H66	Mg30	1.88486	0.95682
H66_1s	Mg30_3s	1.88486	0.91129
H66_1s	Mg30_2p_y	1.88486	0.00016
H66_1s	Mg30_2p_z	1.88486	0.00385

H66_1s	Mg30_2p_x	1.88486	0.04153
Mg18	H74	1.86457	0.91481
Mg18_3s	H74_1s	1.86457	0.8814
Mg18_2p_y	H74_1s	1.86457	-0.00002
Mg18_2p_z	H74_1s	1.86457	0.00226
Mg18_2p_x	H74_1s	1.86457	0.03118

Table S17. Prediction and comparison of the dehydrogenation barriers of the MgH₂/SACs composed of Sc, 4d, and 5d transition metals.

Metal	X_M	θ_d	X	E_a (eV)
3d	Sc	1.36	1	1.080
	Y	1.22	1	1.094
	Zr	1.33	2	2.166
	Nb	1.6	4	4.224
	Mo	2.16	5	5.000
	Tc	1.9	5	5.130
	Ru	2.2	7	6.972
	Rh	2.28	8	7.904
4d	Pd	2.2	10	9.960
	Ag	1.93	10	10.230
	Cd	1.69	10	10.470
	Hf	1.3	2	2.172
	Ta	1.2	3	3.288
	W	2.36	4	3.920
	Re	1.9	5	5.130
	Os	2.2	6	5.976
5d	Ir	2.2	7	6.972
	Pt	2.28	9	8.892
	Au	2.54	10	9.620
				2.653

	Hg	2	10	10.160	2.748
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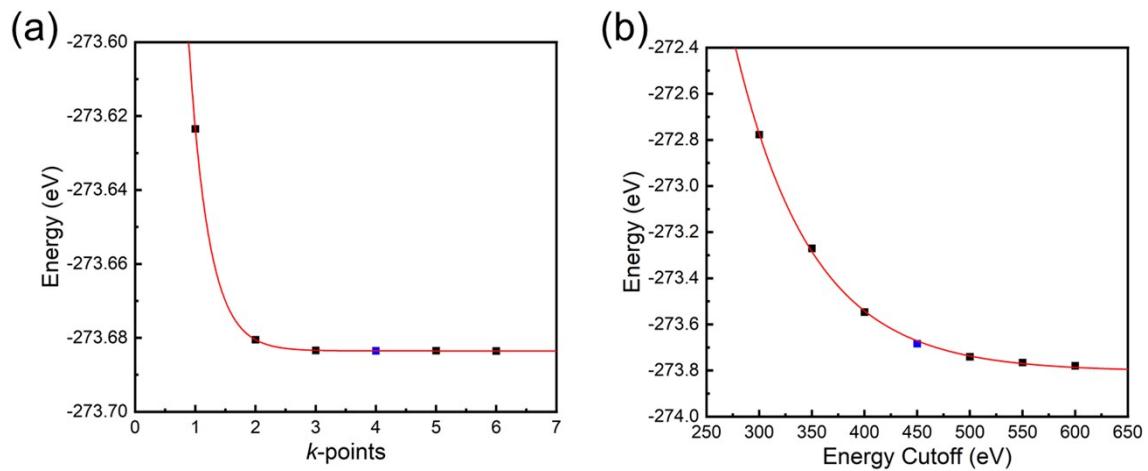


Figure S1. Convergence tests of the calculation settings of (a) k -points and (b) energy cutoff.

The blue points are the k -points and truncation energy selected for our study.

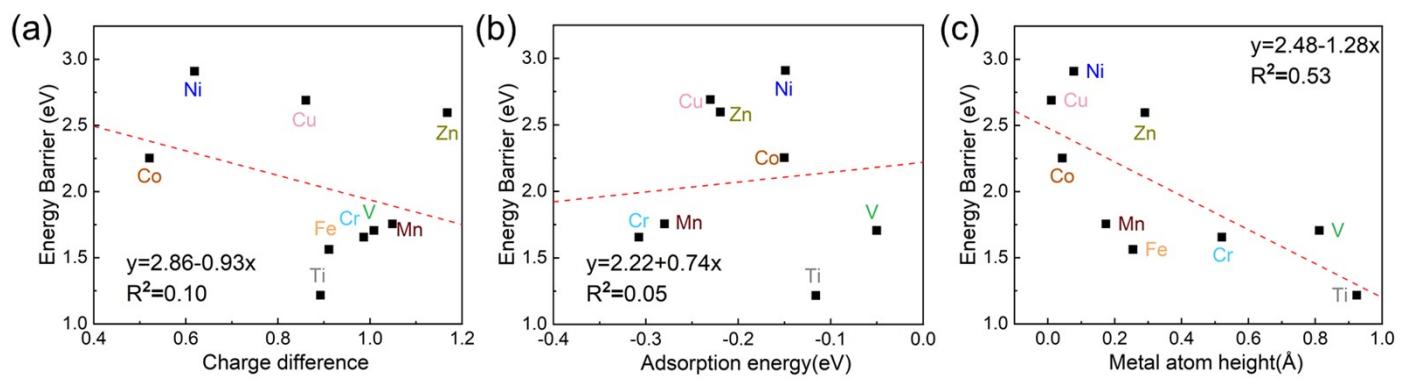


Figure S2. (a) Correlation of charge difference of N vs energy barrier. (b) Correlation of H adsorption energy vs energy barrier. (c) Correlation of metal height vs energy barrier.

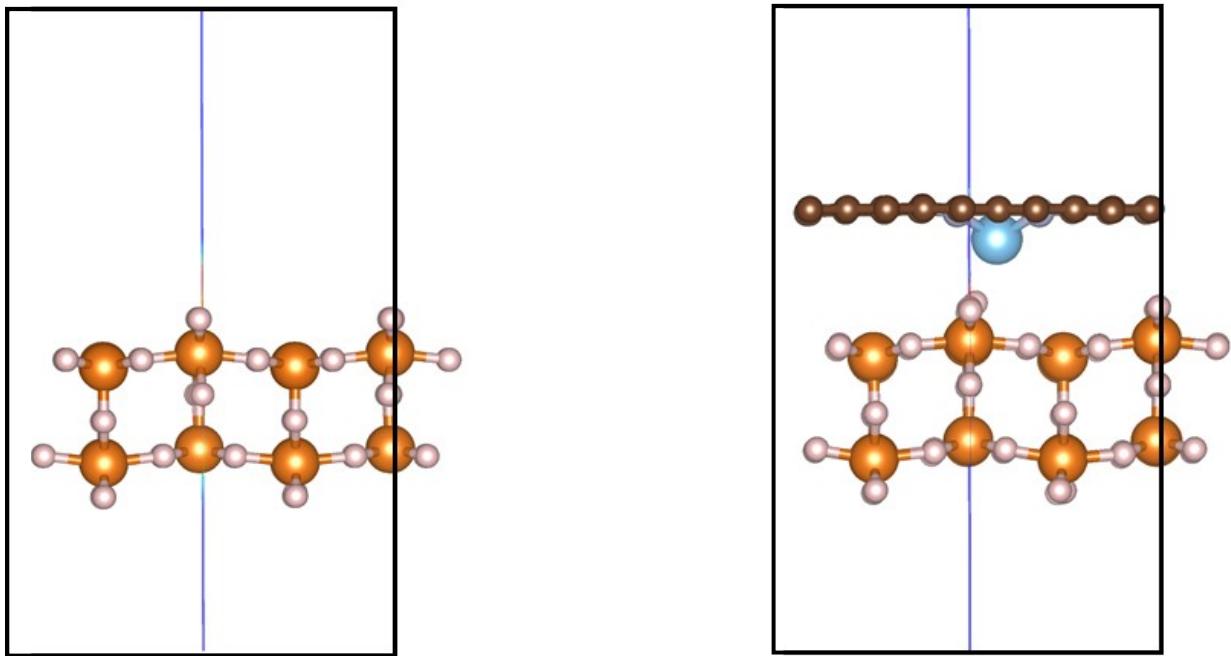


Figure S3. Location of the section for electron localization function analysis.

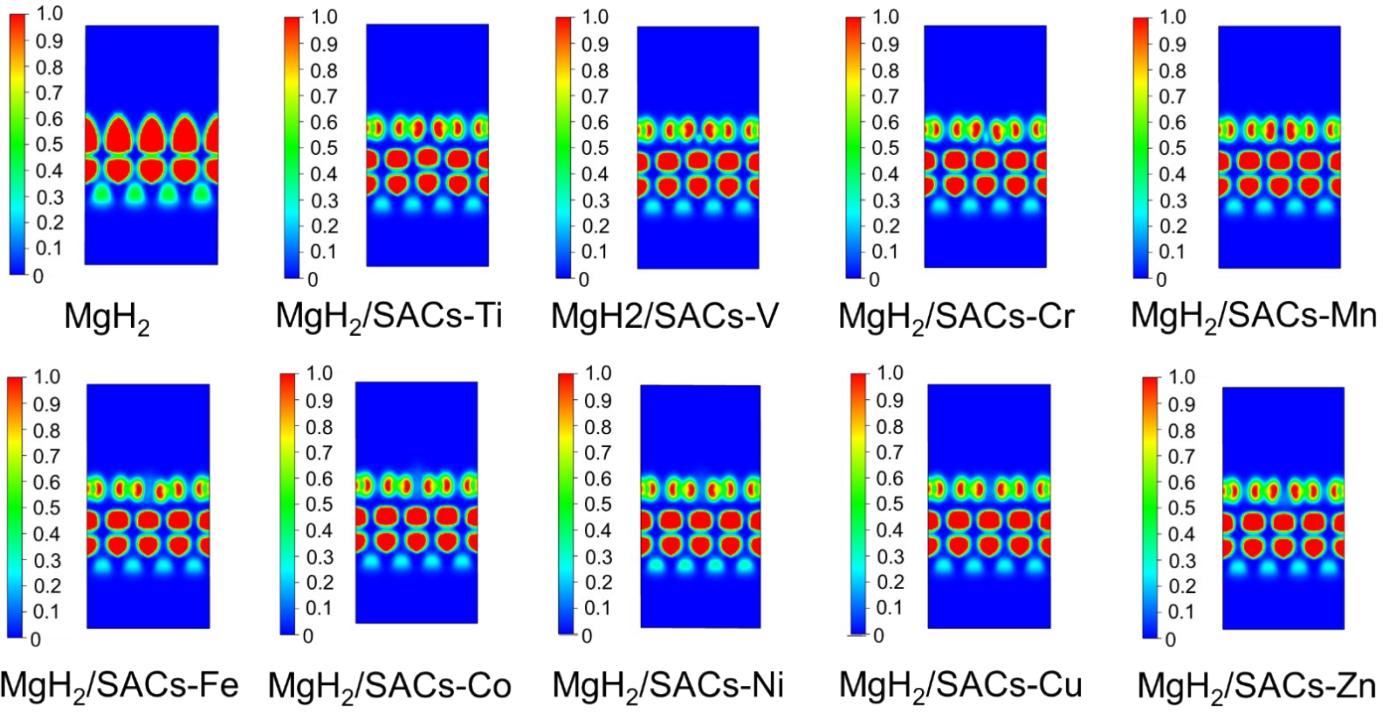


Figure S4. Electron localization functions of MgH_2 and $\text{MgH}_2/\text{SACs-TM}$ (TM = Ti, V, Cr, Mn, Fe, Co, Ni, Cu, and Zn).

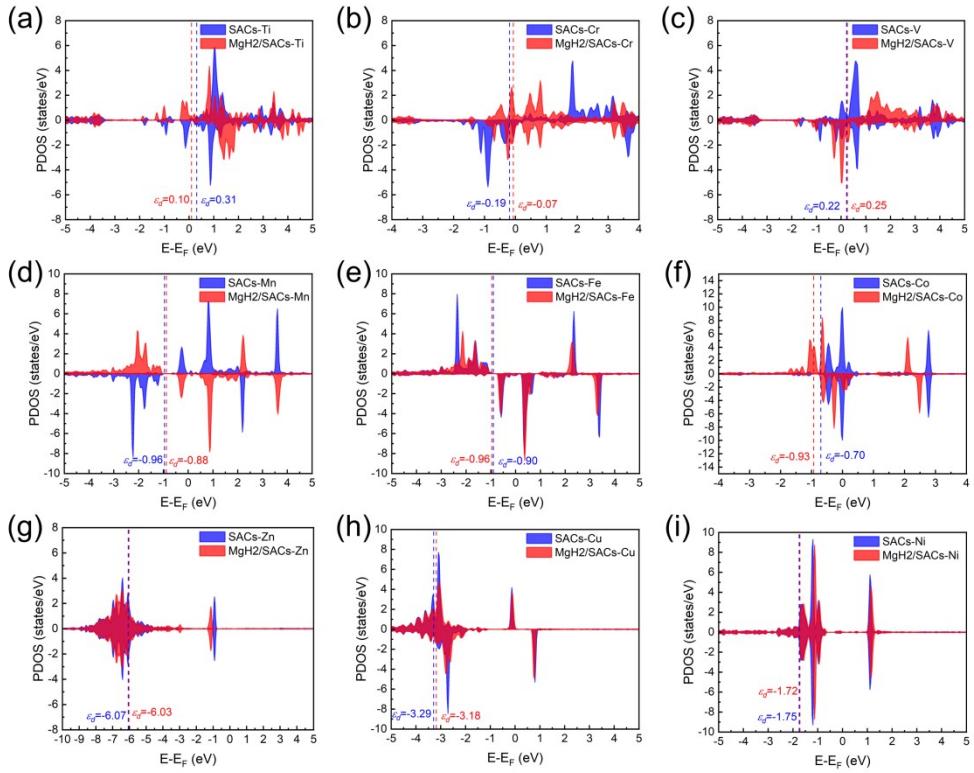


Figure S5. Calculated PDOS of d electrons of the single-atom metal in SACs (in blue) and MgH₂/SACs (in red). All the results are referred to the Fermi level (E_F). The vertical dashed lines represent the calculated average d -band centers.

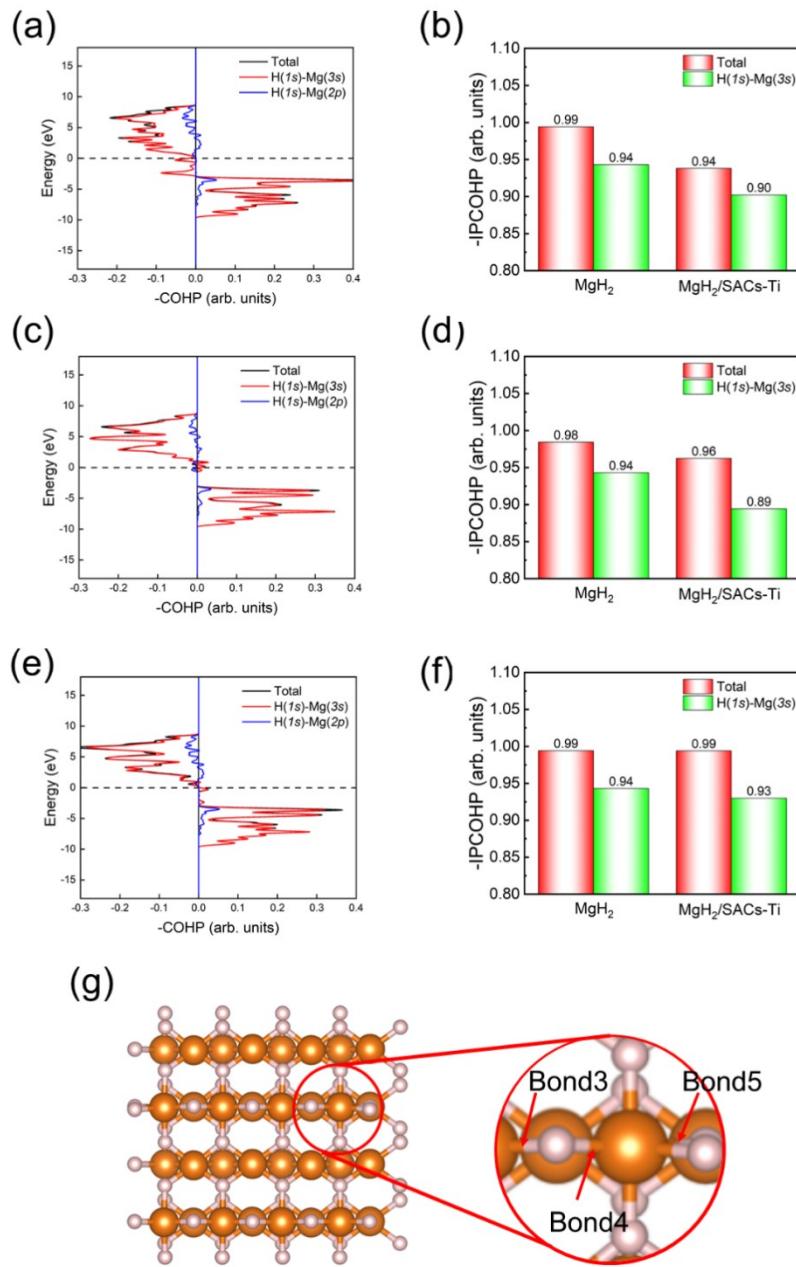


Figure S6. (a, c, e) COHP analysis of the Mg-H Bond3, Bond4, and Bond 5. (b, d, f) Comparison of the integral values of Mg-H Bond3, Bond4, and Bond5 between MgH_2 and $\text{MgH}_2/\text{SACs-Ti}$ in the systems. (g) Illustrations of the Bond3, Bond4, and Bond5 in MgH_2 . White and orange spheres represent H and Mg, respectively.

Atomic Coordinates of Optimized Structures (in VASP POSCAR format)

1. MgH₂

1.000000000000000
11.7980500915556963 -0.0015522264354244 -0.0232039169887414
-0.0016614824187261 12.7077876442912530 0.0187647416700709
-0.0429397505794910 0.0315554332128549 21.2326952059881542

Mg H

32 64

Direct

0.1254185993006682 -0.0005405413579389 0.2918798928495635
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0.7500585761030895 0.4995466977933031 0.2417587612696655
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2. MgH₂/SAC-Ti

1.00000000000000
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 Mg H C N Ti
 32 64 54 4 1
 Direct
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 0.1233210080862401 0.7548791499863217 0.2474350339530014
 0.1231509257927359 0.0049498007366379 0.4025503331428019
 0.9996680385421935 0.0008499851791216 0.2716754706706195
 0.9995253436215665 0.7513220413718374 0.3789196374160503
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 0.3727929000452405 0.0029986085089241 0.4019230456503410
 0.2498079325842224 0.0066942433053760 0.2720770546353967
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0.5953243585734070 0.5308728868172838 0.5678529700325851
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3. MgH₂/SAC-V

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Mg H C N V
32 64 54 4 1
Direct
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0.7492967444836012 0.0059386818547793 0.2703685881681679
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0.1232358007928624 0.0040371494135059 0.4024809472569402
0.9997764202973940 0.0008778884181879 0.2715743536791209
0.9994165880983346 0.7502733949873601 0.3785789680180400
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5. MgH₂/SAC-Mn

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Mg H C N Mn
 32 64 54 4 1

Direct

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6. MgH₂/SAC-Fe

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Mg H C N Fe
32 64 54 4 1
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 0.0498245149839191 0.3254981860624099 0.5708807225867069
 0.7650238111555669 0.2234231821930733 0.5716689579985839
 0.9356568278734371 0.3255673607912131 0.5708237087726632
 0.2181726293795682 0.2230327742869082 0.5715061197218527
 0.1057418473303663 0.2231010094841528 0.5712923220297952
 0.2770275965089312 0.3239528411301313 0.5712173923348912
 0.5470786098082395 0.2184291649977449 0.5748996426294016
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 0.4353337436005070 0.2166015429342169 0.5719015944501598
 0.8780778974176948 0.4240913596793034 0.5709132163222816
 0.0490109841655218 0.5202298533520957 0.5713904976618188

0.7633009434902943 0.4243811712564284 0.5709720058721472
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0.2218805978756990 0.4245577581393876 0.5706670411150854
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0.2787606046073389 0.5269385150642086 0.5678201750227367
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0.8786120741904432 0.6224930846130736 0.5719388941122054
0.0485023676510423 0.7210381585651804 0.5712091084002631
0.7646819692528790 0.6228252470039031 0.5719765992272665
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0.2191220270107868 0.6217506997789433 0.5712645618784976
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0.1054722321463474 0.6212334000864249 0.5715304960414578
0.2658040443143967 0.7234877391991014 0.5713804039733772
0.5477154713042365 0.6287111225345344 0.5711363984583407
0.7105762833647697 0.7232716010954332 0.5714452708542096
0.4358862267105159 0.6286470269742847 0.5699408087334085
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0.3903136715027204 0.5310982739405223 0.5609249004992719
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7. MgH₂/SAC-Co

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-0.0068464808504493 12.2824588188102215 0.0122263271076938
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Mg H C N Co
32 64 54 4 1
Direct

0.8734433842326828 0.7524701714351928 0.2488247475567283
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0.1236394333286628 0.7544988611615782 0.2473778405395410
0.1232358007928644 0.0040371494135069 0.4024809472569410
0.9997764202973908 0.0008778884181892 0.2715743536791185
0.9994165880983378 0.7502733949873595 0.3785789680180379
0.3744022508102908 0.7529998054093443 0.2475628974199378
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0.2495159328183727 0.0066681623222581 0.2704940214511793
0.2489061171289489 0.7553621464685609 0.3797106191966680
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0.6232637141086024 0.0044193463001715 0.4023809218122280
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0.0498451333264603 0.3254369363332762 0.5708333611412939
0.7649237088333920 0.2234646937835937 0.5716455276317199
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0.1057873786292342 0.2230083855943567 0.5712477859172602
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0.5472174779413319 0.2184305103318644 0.5748734486910971
0.7058172387339992 0.3239912726598841 0.5715632132525750
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0.7646632716070255 0.6228843179989620 0.5716271365924293
0.9353980879800781 0.7213332450301689 0.5708715661989409
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0.1055043236835025 0.6211915141676637 0.5714424344608771
0.2660008751381782 0.7233086312053176 0.5713879275079676
0.5478377741070737 0.6287425386001114 0.5711232160220089
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0.5951595217198213 0.5309494288579863 0.5679398212899548
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8. MgH₂/SAC-Ni

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-0.0045792075655624 12.5125013474384570 0.0309755411172287
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Mg H C N Ni
32 64 54 4 1
Direct
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0.7505071470597303 0.0053299803929245 0.2721714479124546
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0.1240438733226360 0.7538945609542307 0.2472610962324479
0.1223936334124194 0.9999539370755021 0.4017934612214697
0.0022374947868766 0.0050129158886224 0.2715809774123816
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9. MgH₂/SAC-Cu

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Mg H C N Cu
32 64 54 4 1

Direct

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10. MgH₂/SAC-Zn

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Mg H C N Zn
32 64 54 4 1

Direct

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