Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

A First-Principles Study on the Thermodynamic and Electronic Properties of Mg and MgH_2 Nanowires

Xinxing Wu,[a] Ruiqi Zhang[a] and Jinlong Yang*[a,b]

[a] Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui 230026, China

[b] Synergetic Innovation Center of Quantum Information & Quantum Physics, University of Science and Technology of China, Hefei, Anhui 230026, China

Table S1. Calculated diameter (D, in nm), lattice parameter along the period direction (c, in Å), and total energy (E, in eV per Mg unit) of Mg(n) nanowires and bulk Mg crystal.

Mg(n)	6	13	24	37	54	73	96	$bulk^{cal}$
D	0.54	0.73	0.96	1.30	1.58	1.92	2.22	
c	3.04	4.84	5.01	5.10	5.11	5.12	5.12	5.18
E	-0.918	-1.055	-1.194	-1.258	-1.306	-1.336	-1.362	-1.524

Table S2. Calculated diameter (D, in nm), lattice parameter along the period direction (c, in Å), total energy (E, in eV per MgH_2 unit), band gap (E_g, in eV), average electron number around Mg atoms (Mg(e), in unit of *e*), average electron number around H atoms (H(e), in unit of *e*), hydrogen desorption energy (ΔE_d, in eV/H_2 and kJ/mol H_2) and hydrogen desorption temperature (T_d, in K) of MgH_2(n) nanowires and bulk MgH_2 crystal. The experimental hydrogen desorption enthalpy ΔH_d of bulk MgH_2 crystal is 0.777 eV/H_2 (75.0 kJ/mol H_2). 1 eV/H_2 = 96.485 kJ/mol H_2.

MgH_2(n)	6	13	24	37	54	73	96	$bulk^{cal}$	$bulk^{exp}$
D	0.63	0.87	1.25	1.56	1.94	2.25	2.63		
c	5.99	6.23	6.31	6.29	6.31	6.34	6.35	6.37	6.37
E	-8.147	-8.338	-8.537	-8.629	-8.693	-8.727	-8.761	-8.975	
E_g	3.26	2.40	2.47	2.25	2.29	1.95	1.97	3.77	5.6
Mg(e)	0.474	0.456	0.446	0.439	0.438	0.436	0.436	0.416	
H(e)	1.763	1.772	1.777	1.780	1.781	1.782	1.782	1.792	
ΔE_d[a]	0.439	0.493	0.553	0.582	0.597	0.602	0.609	0.661	0.777
ΔE_d[b]	42.4	47.6	53.3	56.1	57.6	58.0	58.8	63.8	75.0
T_d	324	364	408	429	440	444	450	488	574

[a] eV/H_2. [b] kJ/mol H_2.

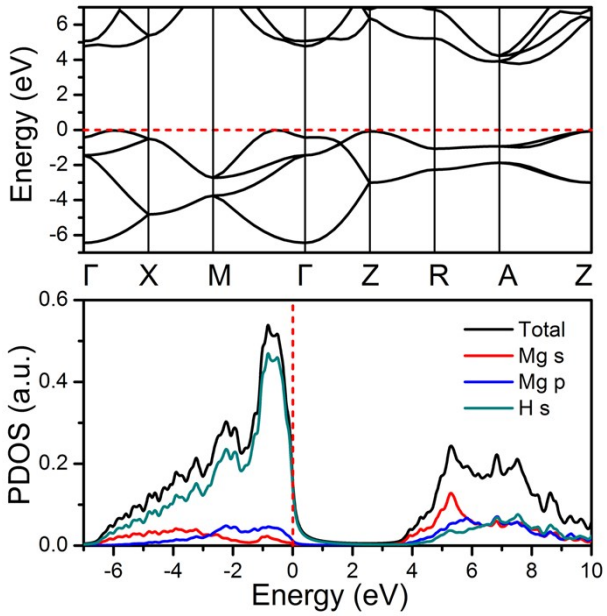

Figure S1. Band structure and density of state (DOS) of bulk MgH_2 crystal. The Fermi level is set to zero by red dashed line.

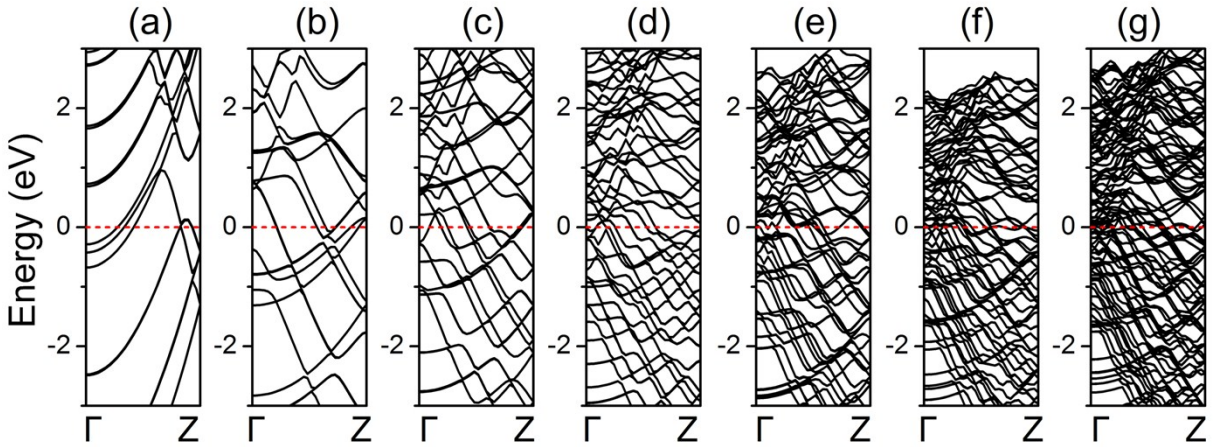

Figure S2. Band structures of Mg nanowires: (a) Mg(6), (b) Mg(13), (c) Mg(24), (d) Mg(37), (e) Mg(54), (f) Mg(73), (g) Mg(96) nanowire. The Fermi level is set to zero by red horizontal line.

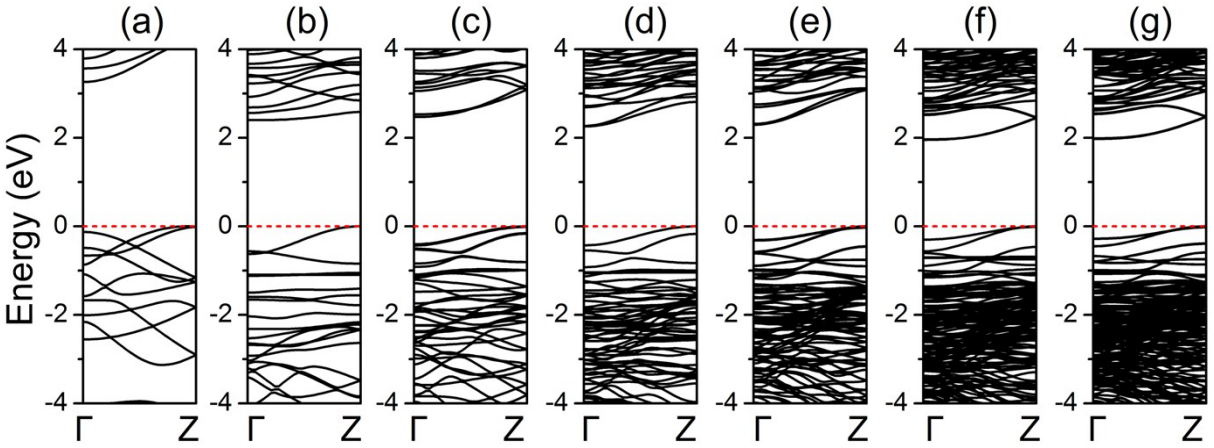

Figure S3. Band structures of MgH_2 nanowires: (a) MgH_2(6), (b) MgH_2(13), (c) MgH_2(24), (d) MgH_2(37), (e) MgH_2(54), (f) MgH_2(73), (g) MgH_2(96) nanowire. The Fermi level is set to zero by red horizontal line.

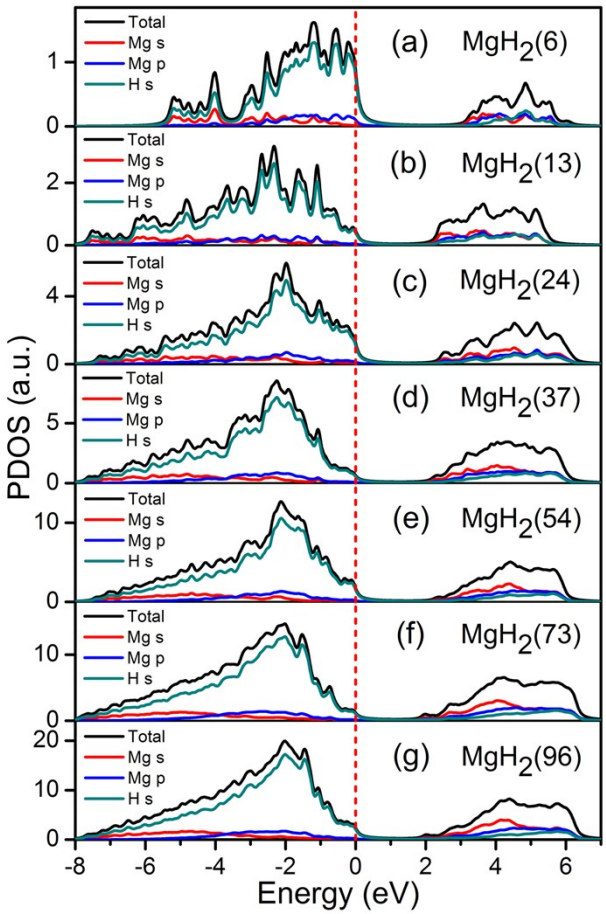

Figure S4. Partial density of states (PDOS) of MgH_2 nanowires. The Fermi level is set to zero by red vertical line.