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Electronic Supporting Information

Fast hydride-ion conduction in complex hydride Ba_2MgH_6

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Table S1. Refined crystal structure parameters of Ba_2MgH_6 obtained from the room-temperature synchrotron X-ray diffraction (SXRD) pattern.

Atom	Wyckoff position	*g*	*x*	*y*	*z*	B_{Iso}/ Å^2
Ba	2*d*	1	0.333333	0.666667	0.7336(2)	0.827(6)
Mg	1*a*	1	0	0	0	0.37(7)
H2	6*i*	1	0.1573(17)	0.315(3)	0.311(9)	1.2(6)

Unit cell: Trigonal *P*-3*m*1 (164); a = 5.730901(14) Å, c = 4.51870(3) Å, R_{wp} = 4.82 %, R_e = 2.62%, R_p = 3.58%, R_B = 6.40%, R_F = 4.20%, goodness of fit $S = R_{wp}/R_e$ = 1.84

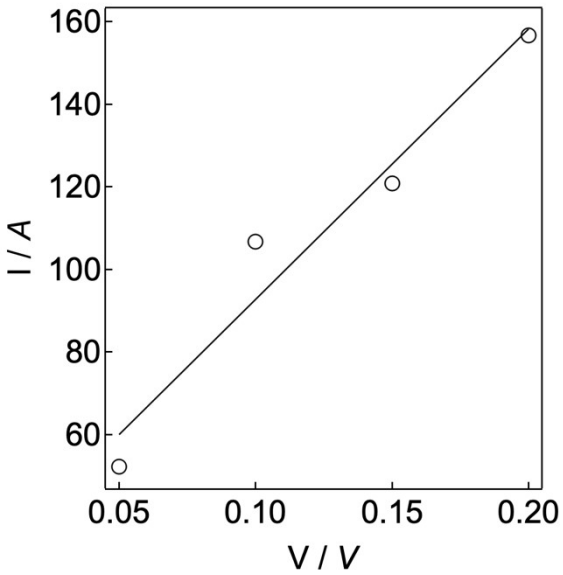

Figure S1. *I–V* characteristics of Ba_2MgH_6 obtained by the DC polarization method at 661 K.

Table S2. Reliability factors, phase fractions, and Ba-site occupancies obtained from Rietveld refinement of the SXRD data.

Temp (K)	Reliability factors						Phase fractions			*g* (Ba)
	S	R_{wp}	R_p	R_e	R_B	R_F	Ba_2MgH_6	BaH_2	MgH_2	
300.0	1.67	4.37	3.41	2.61	7.08	4.26	0.957(1)	0.0000(5)	0.0428(14)	0.989(5)
363.3	1.66	4.34	3.41	2.62	3.87	2.81	0.939(1)	0.0110(5)	0.0500(14)	0.985(5)
459.3	1.55	4.08	3.24	2.63	4.45	3.42	0.915(2)	0.0165(5)	0.0688(17)	0.963(5)
561.1	1.69	4.45	3.53	2.63	6.47	4.93	0.906(2)	0.0196(5)	0.0743(18)	0.962(6)
622.6	1.63	4.31	3.36	2.65	5.87	3.85	0.877(2)	0.0465(8)	0.0767(20)	0.955(6)
643.0	1.62	4.30	3.29	2.65	5.27	3.91	0.866(2)	0.0817(11)	0.0519(14)	0.944(6)
653.1	1.57	4.16	3.20	2.65	4.98	3.21	0.815(2)	0.1238(15)	0.0607(17)	0.940(9)
663.2	1.55	4.12	3.22	2.66	6.00	4.00	0.811(2)	0.1527(17)	0.0365(16)	0.935(6)
673.3	1.72	4.59	3.61	2.66	6.28	6.62	0.761(3)	0.1958(21)	0.0428(15)	0.938(6)
683.3	1.54	4.07	3.15	2.65	5.04	3.78	0.721(3)	0.2411(23)	0.0378(14)	0.934(6)
703.3	1.66	4.42	3.33	2.65	4.99	4.01	0.704(3)	0.2720(25)	0.0238(10)	0.922(6)
733.0	1.86	4.97	3.86	2.66	7.12	6.11	0.670(4)	0.292(4)	0.0376(15)	0.915(8)
762.3	2.23	5.94	4.34	2.66	8.40	5.73	0.6335(9)	0.3438(7)	0.0227(11)	0.897(6)

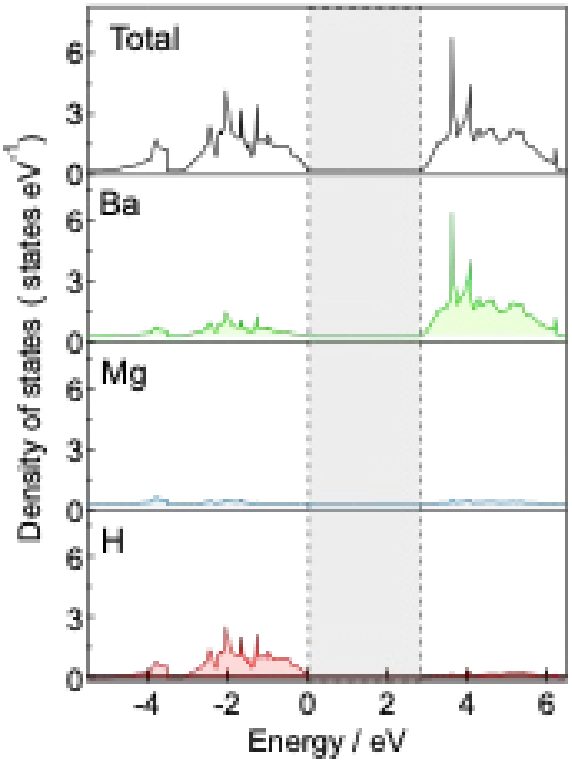

Figure S2. Calculated electronic density of states (DOS) of Ba_2MgH_6.

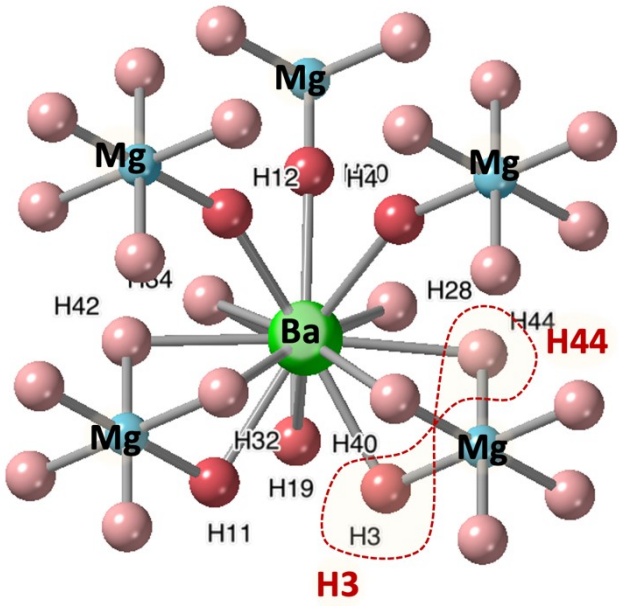

Figure S3. Inequivalent anion sites in Ba_2MgH_6, with hydrogen atoms represented by pink and dark pink spheres. The green and blue spheres represent Ba and Mg, respectively. The Schottky defect with the lowest energy corresponds to hydrogen vacancies at the H3 and H44 sites, highlighted by red dashed lines.

Table S3. Relative energies of hydrogen vacancy (V_H) pairs in Ba_2MgH_6. The numbering of hydrogen sites is illustrated in Fig, S3.

V_H pairs	Relative energy *E* / eV
H12H4	0.0693
H3H11	0.1010
H3H12	0.0371
H3H4	0.1540
H44H11	0.0455
H44H12	0.0174
H44H19	0.0419
H44H20	0.0226
H44H28	0.0136
H44H3	0.0000
H44H34	0.0797
H44H4	0.0979
H44H42	0.1780

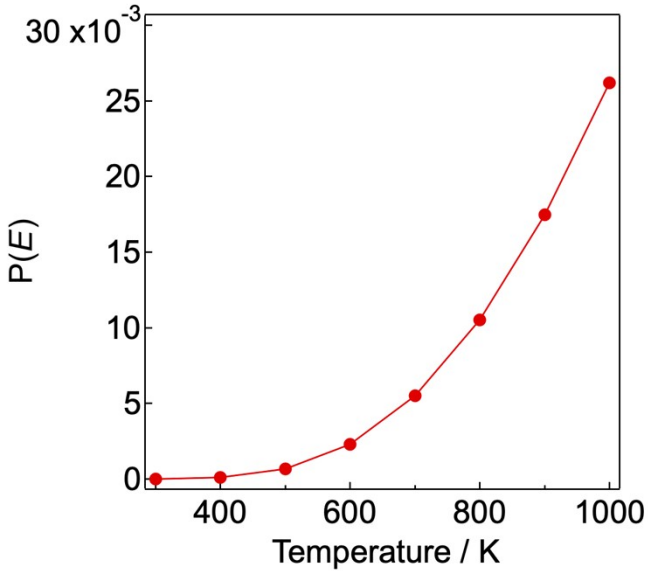

Figure S4. Probability $P(E)$ of Schottky defect formation in $Ba_{1.875}MgH_{5.75}$, calculated as $P(E) = \exp(-E/kT)$, where E is the formation energy, k is the Boltzmann constant, and T is the absolute temperature.

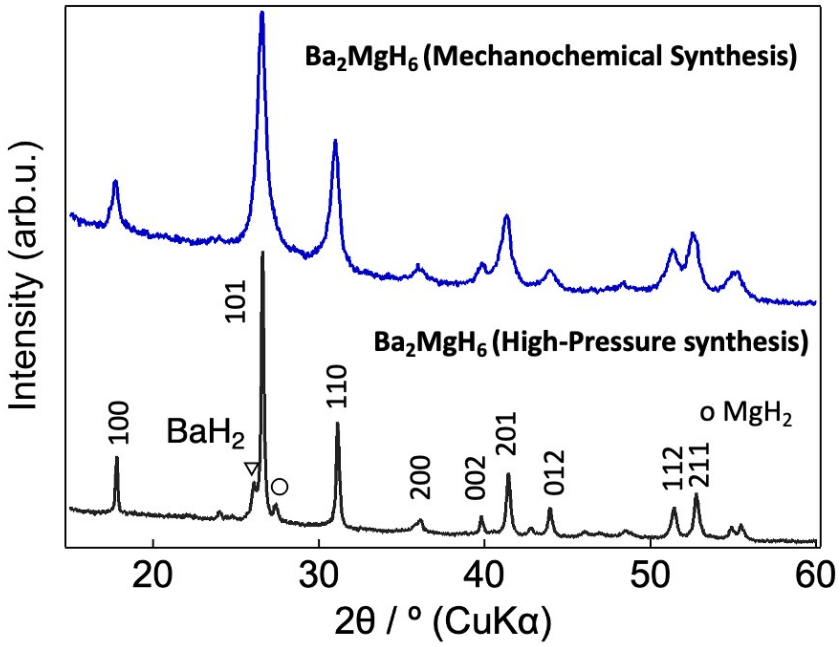

Figure S5. XRD patterns of Ba_2MgH_6 prepared by mechanochemical synthesis (top) and high-pressure synthesis (bottom). Triangle and circle markers indicate diffraction peaks from BaH_2 and MgH_2 impurities, respectively.

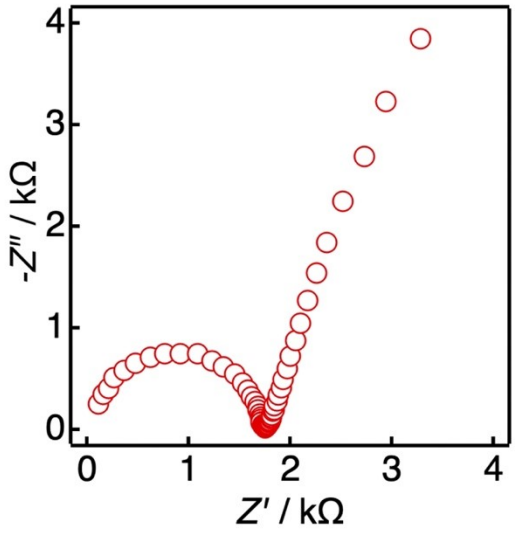

Figure S6. Nyquist plot of mechanochemically synthesized Ba_2MgH_6 recorded at 473 K.