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Supporting Information

Tailoring the d-band center by borophene subunits in chromic diboride toward the hydrogen evolution reaction

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Keywords: Chromic diboride, d-band center, borophene subunits, hydrogen evolution reaction, high pressure and high temperature, electrocatalyst.

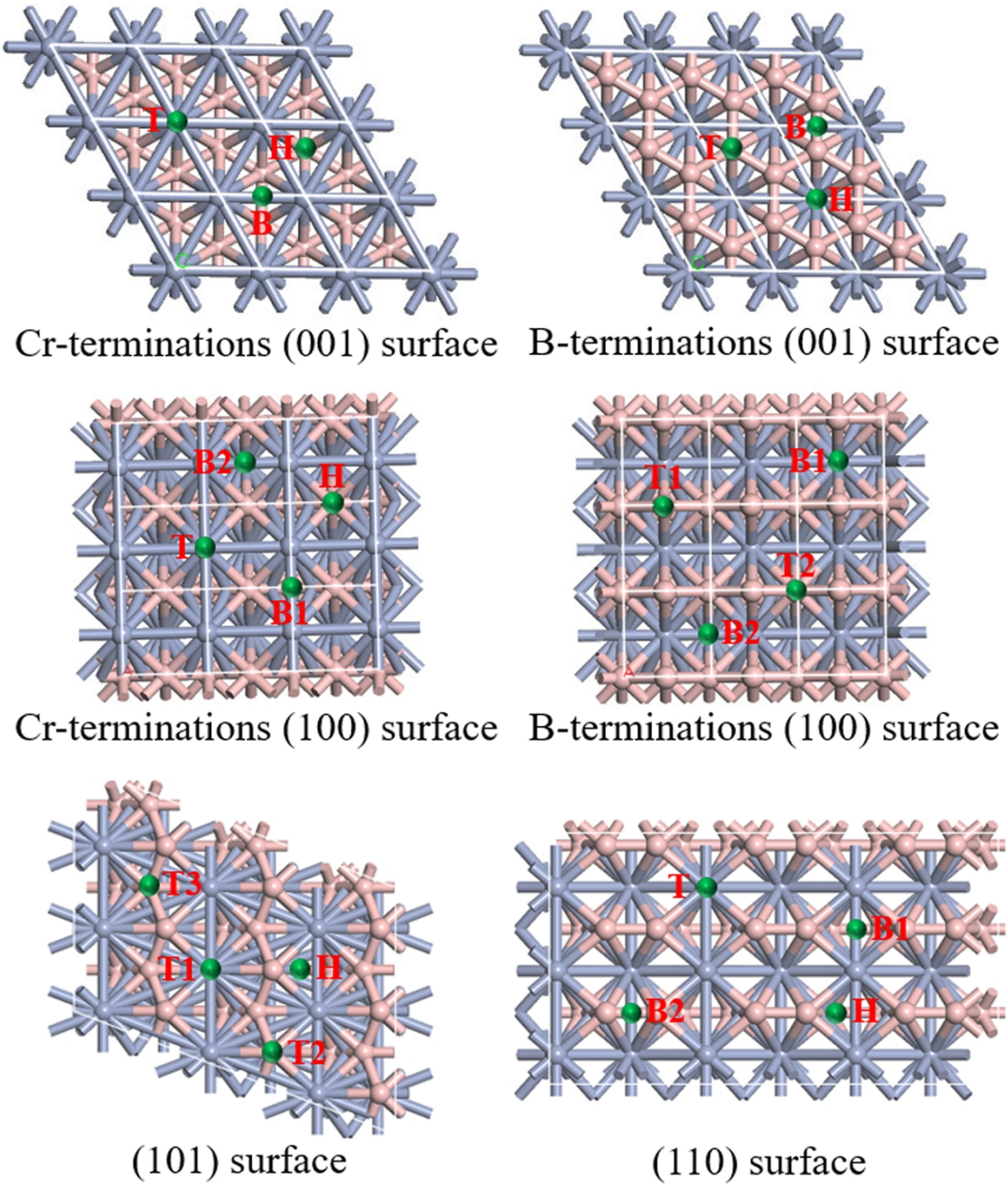

Figure S 1. The possible adsorption sites for H* in CrB_2. Here, the top, bridge and hollow sites are denoted with "T", "B" and "H", respectively. Cr, B and H atoms are marked with the pink, grey and green spheres, respectively.

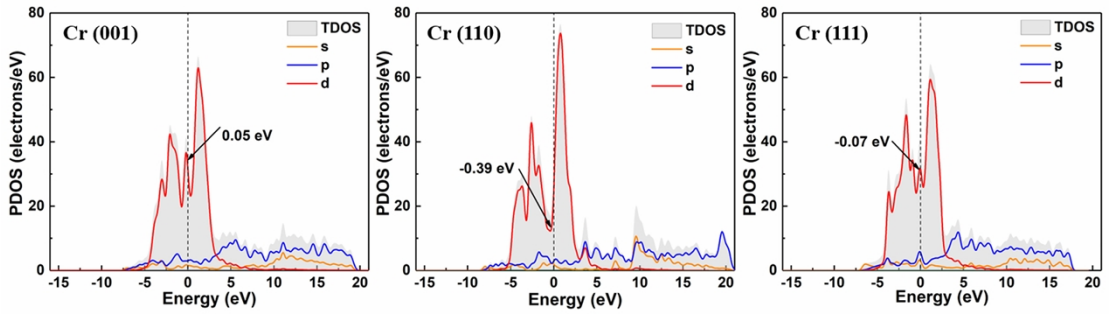

Figure S 2. The projected density of states (PDOS) for metallic Cr in (a) (001), (b) (110) and (c) (111) surface. The line of dashes denotes the position of the Fermi energy, and the arrows indicate the sites of d-band centers.

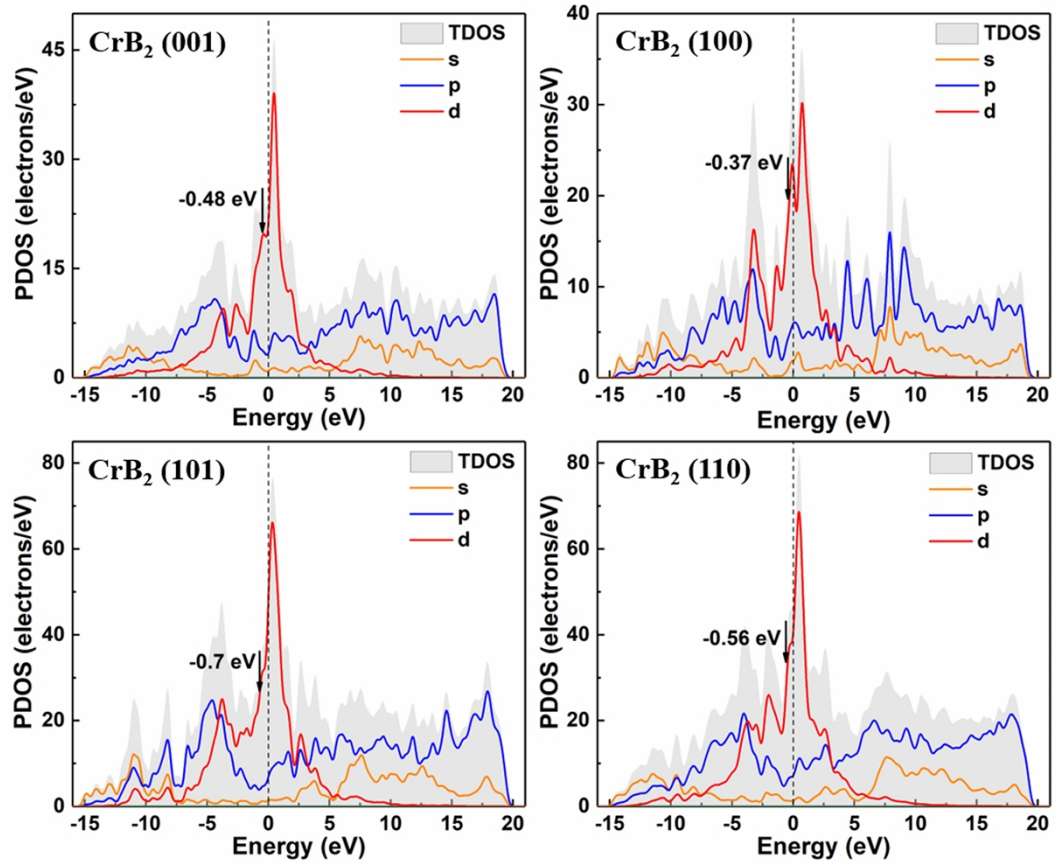

Figure S 3. The projected density of states (PDOS) for CrB_2 in (a) (001), (b) (100), (c) (101) and (d) (110) surface. The line of dashes denotes the position of the Fermi energy, and the arrows indicate the sites of d-band centers.

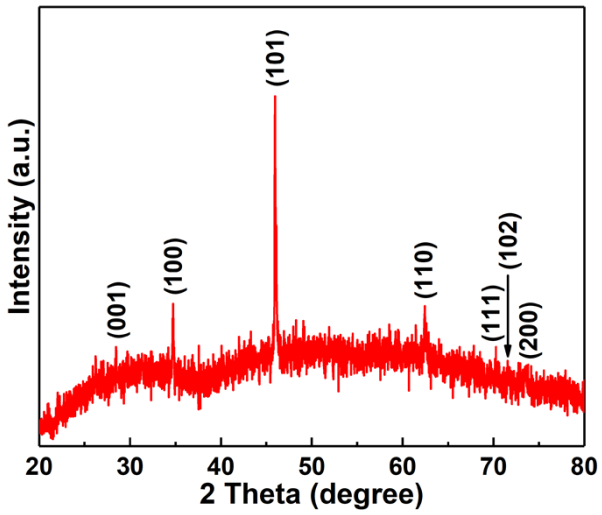

Figure S 4. XRD pattern of CrB_2 after long time HER in 0.5 M H_2SO_4 solution.

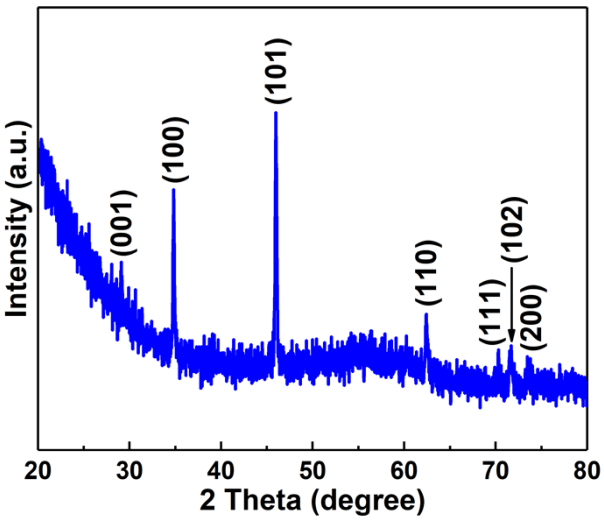

Figure S 5. XRD pattern of CrB_2 after long time HER in 1 M KOH solution.

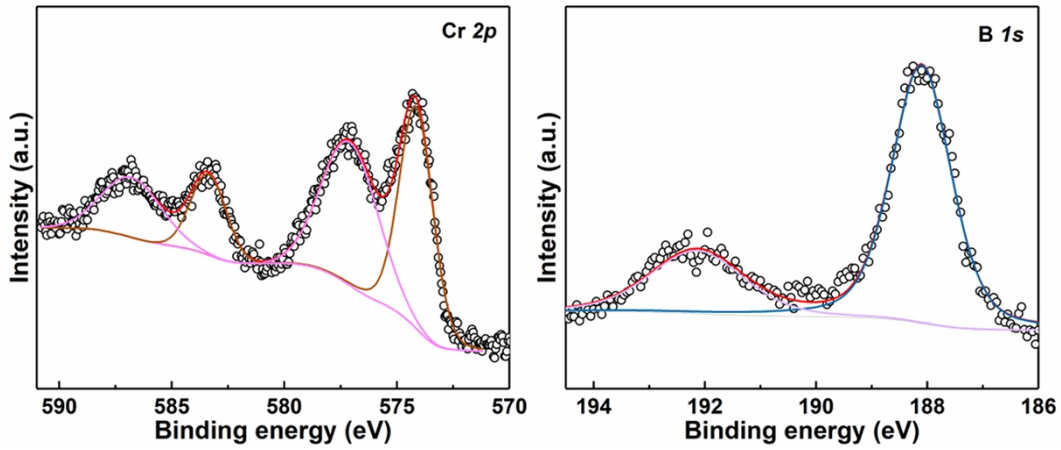

Figure S 6. The XPS of CrB_2 after long time HER in 0.5 M H_2SO_4 solution.

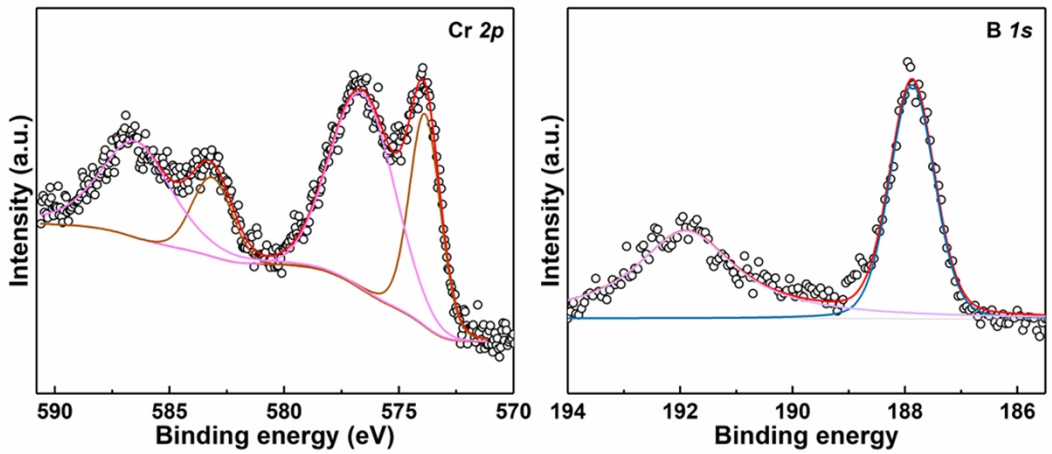

Figure S 7. The XPS of CrB_2 after long time HER in 1 M KOH solution.

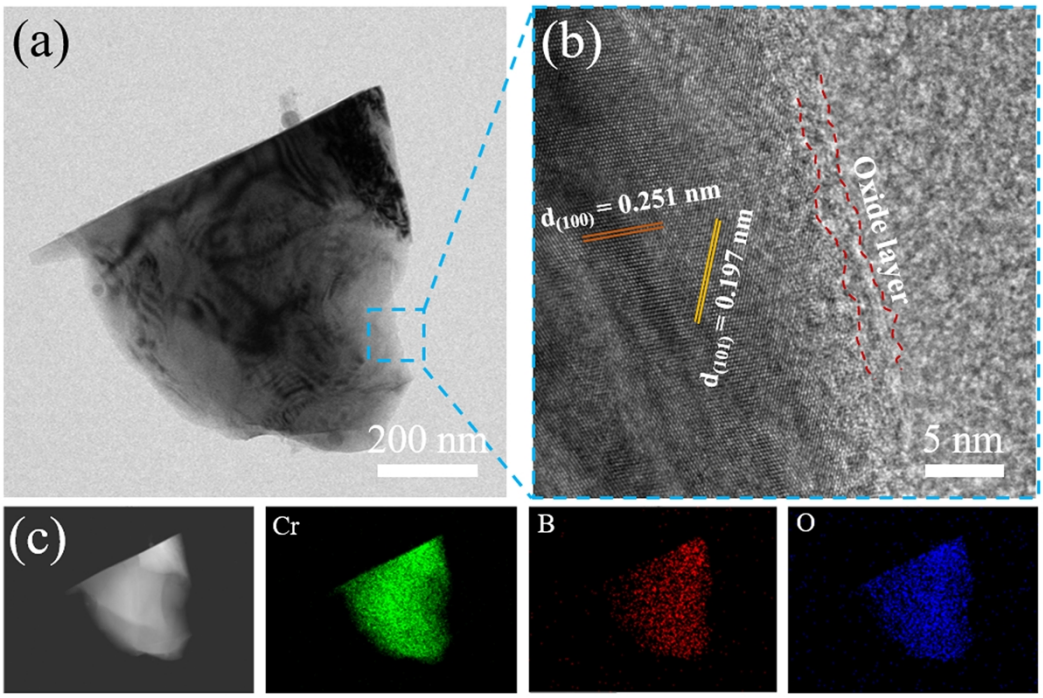

Figure S 8. (a) TEM, (b) HRTEM, and (c) EDX elemental maps of CrB_2 after long time HER in 0.5 M H_2SO_4 solution.

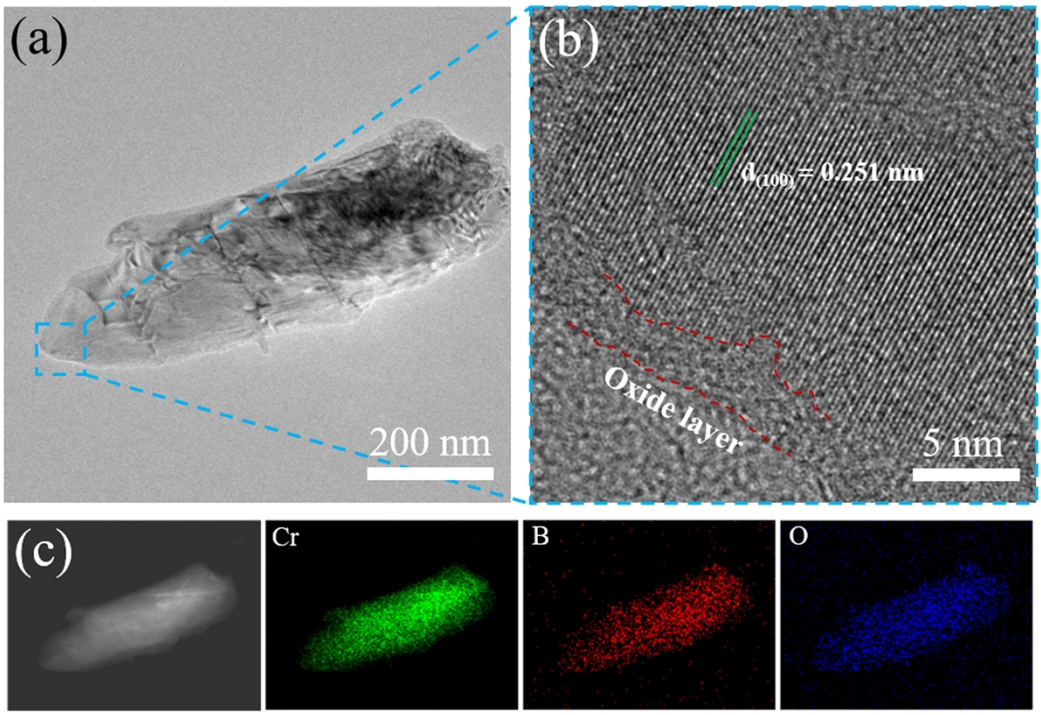

Figure S 9. (a) TEM, (b) HRTEM, and (c) EDX elemental maps of CrB_2 after long time HER in 1 M KOH solution.

Table S1. Calculated the Gibbs free energy (ΔG_{H^*}) of H adsorption (25 % H coverage) on different surfaces of CrB_2.

	Cr-terminated (001)	B-terminated (001)	Cr-terminated (100)	B-terminated (100)	(101)	(110)
T/T1	-0.14	-0.04	0.21	-0.69	0.48	0.45
T2	--	--	--	0.57	*	--
T3	--	--	--	--	*	--
B/B1	-0.43	-0.35	-0.07	0.58	--	0.26
B2	--	--	-0.22	1.43	--	-0.05
H	-0.48	1.53	-0.08	--	0.04	-0.46

* The absorption site eventually deviates from its original position, and optimized to the H site.

Table S2. Calculated the Gibbs free energy (ΔG_{H^*}) of H adsorption (25 % H coverage) on different surfaces of metallic Cr.

	(001)	(110)	(111)
T	0.21	0.16	0.71
B	-0.4	-0.23	-0.54
H	-0.51	-0.52	-0.54