Electronic Supplementary Material

Bilayer borophene: an efficient catalyst for hydrogen evolution reaction

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Table S1 The change in ΔE_{H^*} of H atom at different possible adsorption sites, the distance between H atom and adsorption point B atom before and after adsorption of H atom, and the number of electrons obtained by H atom on the structure of BL-α borophene.

BL-α borophene		**B-H Bond length/Å**		**ΔQ/e**
Sites (Top)	Energy (ΔE_{H^*})	initial	final	
1	–0.48	1.60	1.21	0.414
2	–0.49	1.59	1.22	0.410
3	0.48	1.60	1.21	0.538
4	–0.49	1.60	1.21	0.413
5	–0.49	1.60	1.22	0.412

Table S2 The change in ΔE_{H^*} of H atom at different possible adsorption sites, the distance between H atom and adsorption point B atom before and after adsorption of H atom, and the number of electrons obtained by H atom on the structure of BL-β borophene.

BL-β borophene		**B-H Bond length/Å**		**ΔQ/e**
Sites (Top)	Energy (ΔE_{H^*})	initial	final	
m	0.26	1.60	1.21	0.475
1	–0.45	1.60	1.21	0.478
2	–0.22	1.60	1.30	0.338
3	–0.16	1.60	1.22	0.497

4	–0.22	1.60	1.22	0.490
5	–0.26	1.60	1.22	0.486
Sites (Bridge)	Energy (ΔE_{H^*})	initial	final	
m-1	–0.44	1.60	1.21	0.482
m-2	–0.29	1.60	1.31	0.389
m-3	–0.15	1.60	1.22	0.493
m-4	0.23	1.60	1.22	0.424
m-5	–0.22	1.60	1.22	0.478
m-6	0.05	1.60	1.22	0.428
1-2	–0.3	1.60	1.23	0.396
1-3	0.08	1.60	1.23	0.418
1-4	–0.44	1.60	1.22	0.492
1-5	0.05	1.60	1.22	0.428
2-3	–0.16	1.59	1.22	0.498
2-4	0.17	1.60	1.28	0.630
3-3	–0.08	1.60	1.22	0.460
3-4	–0.16	1.60	1.22	0.496
3-5	–0.16	1.60	1.22	0.484
4-3	–0.05	1.60	1.23	0.437
4-4	–0.22	1.60	1.23	0.484
4-5	–0.22	1.60	1.22	0.485

Table S3 The change in ΔE_{H^*} of H atom at different possible adsorption sites, the distance between H atom and adsorption point B atom before and after adsorption of H atom, and the number of electrons obtained by H atom on the structure of BL-i borophene.

BL-i borophene		**B-H Bond length/Å**		**ΔQ/e**
Sites (Top)	Energy (ΔE_{H^*})	initial	final	
1	–0.51	1.60	1.21	0.522
2	–0.01	1.60	1.31	0.552
3	–0.24	1.60	1.22	0.525
4	–0.51	1.60	1.22	0.521
5	–0.14	1.60	1.37	0.531
6	0.05	1.60	1.22	0.566
Sites (Bridge)	Energy (ΔE_{H^*})	initial	final	
1-2	–0.01	1.60	1.22	0.555
1-4	–0.01	1.60	1.22	0.557
2-3	–0.24	1.60	1.23	0.522
2-4	–0.51	1.60	1.23	0.521
3-4	–0.51	1.60	1.22	0.521
3-5	–0.24	1.60	1.22	0.520
3-6	0.13	1.59	1.22	0.408
4-5	–0.51	1.60	1.21	0.521

4-6	–0.51	1.60	1.22	0.521
5-6	–0.51	1.60	1.22	0.519

Table S4 The change in ΔE_{H^*} of H atom at different possible adsorption sites, the distance between H atom and adsorption point B atom before and after adsorption of H atom, and the number of electrons obtained by H atom on the structure of BL-m borophene.

BL-m borophene		**B-H Bond length/Å**		**ΔQ/e**
Sites (Top)	Energy (ΔE_{H^*})	initial	final	
1	–0.59	1.60	1.22	0.409
2	–0.60	1.60	1.20	0.395
3	–0.66	1.59	1.32	0.463
4	–0.56	1.60	1.32	0.468
5	0.01	1.60	1.21	0.403
6	–0.56	1.60	1.39	0.491
7	–0.56	1.60	1.32	0.458
8	–0.56	1.60	1.32	0.467

Table S5 The change in ΔE_{H^*} of H atom at different possible adsorption sites, the distance between H atom and adsorption point B atom before and after adsorption of H atom, and the number of electrons obtained by H atom on the structure of BL-n borophene.

BL-n borophene		**B-H Bond length/Å**		**ΔQ/e**
Sites (Top)	Energy (ΔE_{H^*})	initial	final	
1	0.24	1.60	1.20	0.372
2	–0.08	1.59	1.22	0.437
3	–0.86	1.60	1.34/1.36	0.459
4	–0.60	1.60	1.23	0.366
5	–0.85	1.60	1.34/1.36	0.452

Table S6 The change in ΔE_{H^*} of H atom at different possible adsorption sites, the distance between H atom and adsorption point B atom before and after adsorption of H atom, and the number of electrons obtained by H atom on the structure of BL-s borophene.

BL-s borophene	**B-H Bond length/Å**	**ΔQ/e**

Sites (Top)	Energy (ΔE_{H^*})	initial	final	
1	–0.20	1.60	1.24	0.403
2	–0.29	1.60	1.37	0.534
3	0.51	1.59	1.21	0.449
4	–0.20	1.60	1.30	0.403
5	–0.20	1.60	1.21	0.417
6	0.50	1.60	1.22	0.456
Sites (Bridge)	Energy (ΔE_{H^*})	initial	final	
1-2	–0.20	1.60	1.21	0.404
1-3	–0.20	1.60	1.20	0.404
1-4	0.17	1.59	1.23	0.414
1-6	–0.19	1.60	1.21	0.408
2-3	–0.20	1.60	1.22	0.410
3-4	–0.19	1.60	1.21	0.401
4-5	–0.28	1.60	1.23	0.531
4-6	–0.19	1.60	1.21	0.404
5-6	–0.19	1.60	1.22	0.406

Table S7 The change in ΔE_{H^*} of H atom at different possible adsorption sites, the distance between H atom and adsorption point B atom before and after adsorption of H atom, and the number of electrons obtained by H atom on the structure of BL-t borophene.

BL-t borophene		**B-H Bond length/Å**		**ΔQ/e**
Sites (Top)	Energy (ΔE_{H^*})	initial	final	
1	0.20	1.60	1.22	0.391
2	1.12	1.60	1.23	0.355
3	1.12	1.60	1.22	0.355
4	0.22	1.60	1.22	0.427
5	0.23	1.60	1.22	0.416

Table S8 The adsorption energy, Zero-point energy (ZPE), entropic corrections (TS) at T=298 K to the free energies and (ZPE–TS) values of the adsorbed species (with*) on the structure of BL-α borophene. The Zero-point energy (ZPE) and entropic corrections (TS) to the free energies values were obtained by calculating the vibration frequency of the reaction intermediate.

BL-α-Top	ΔE_{H^*}/eV	ZPE/eV	*TS*/eV	ZPE – *TS*/eV
1	–0.48	0.236	0.003	0.232

2	–0.49	0.235	0.004	0.232
3	0.48	0.245	0.006	0.240
4	–0.49	0.236	0.003	0.232
5	–0.49	0.235	0.003	0.232

Table S9 The adsorption energy, Zero-point energy (ZPE), entropic corrections (TS) at T=298 K to the free energies and (ZPE–TS) values of the structure of BL-β borophene.

BL-β-Top	ΔE_{H^*}/eV	ZPE/eV	*TS*/eV	ZPE – *TS*/eV
m	0.26	0.247	0.005	0.242
1	–0.45	0.246	0.005	0.241
2	–0.22	0.215	0.006	0.209
3	–0.16	0.247	0.005	0.242
4	–0.22	0.238	0.006	0.232
5	–0.26	0.234	0.007	0.227
BL-β-Bridge	ΔE_{H^*}/eV	ZPE/eV	*TS*/eV	ZPE – *TS*/eV
m-1	–0.44	0.246	0.005	0.241
m-2	–0.29	0.229	0.004	0.225
m-3	–0.15	0.247	0.005	0.243
m-4	0.23	0.224	0.009	0.214
m-5	–0.22	0.234	0.007	0.227
m-6	0.05	0.227	0.009	0.219
1-2	–0.3	0.216	0.012	0.204
1-3	0.08	0.230	0.008	0.221
1-4	–0.44	0.246	0.005	0.241
1-5	0.05	0.227	0.009	0.219
2-3	–0.16	0.247	0.005	0.242
2-4	0.17	0.237	0.007	0.230
3-3	–0.08	0.240	0.006	0.234

3-4	–0.16	0.247	0.005	0.242
3-5	–0.16	0.247	0.005	0.242
4-3	–0.05	0.228	0.004	0.224
4-4	–0.22	0.238	0.006	0.232
4-5	–0.22	0.238	0.006	0.232

Table S10 The adsorption energy, Zero-point energy (ZPE), entropic corrections (TS) at T=298 K to the free energies and (ZPE–TS) values of the structure of BL-i borophene.

BL-i-Top	ΔE_{H^*}/eV	ZPE/eV	*TS*/eV	ZPE – *TS*/eV
1	–0.51	0.248	0.006	0.241
2	–0.01	0.240	0.008	0.232
3	–0.24	0.244	0.006	0.238
4	–0.51	0.248	0.006	0.242
5	–0.14	0.232	0.003	0.228
6	0.05	0.241	0.008	0.233
BL-i-Bridge	ΔE_{H^*}/eV	ZPE/eV	*TS*/eV	ZPE – *TS*/eV
1-2	–0.01	0.240	0.008	0.232
1-4	–0.01	0.241	0.008	0.232
2-3	–0.24	0.244	0.006	0.238
2-4	–0.51	0.248	0.006	0.242
3-4	–0.51	0.248	0.006	0.242
3-5	–0.24	0.244	0.006	0.238
3-6	0.13	0.228	0.004	0.225
4-5	–0.51	0.248	0.006	0.242
4-6	–0.51	0.248	0.006	0.242
5-6	–0.51	0.248	0.006	0.242

Table S11 The adsorption energy, Zero-point energy (ZPE), entropic corrections (TS) at T=298 K to the free energies and (ZPE–TS) values of the structure of BL-m borophene.

BL-m-Top	ΔE_{H^*}/eV	ZPE/eV	*TS*/eV	ZPE – *TS*/eV
1	–0.59	0.229	0.009	0.220
2	–0.60	0.227	0.010	0.218
3	–0.66	0.235	0.003	0.232
4	–0.56	0.238	0.003	0.234
5	0.01	0.238	0.007	0.232
6	–0.56	0.238	0.003	0.235
7	–0.56	0.238	0.003	0.234
8	–0.56	0.238	0.003	0.234

Table S12 The adsorption energy, Zero-point energy (ZPE), entropic corrections (TS) at T=298 K to the free energies and (ZPE–TS) values of the structure of BL-n borophene.

BL-n-Top	ΔE_{H^*}/eV	ZPE/eV	*TS*/eV	ZPE – *TS*/eV
1	0.24	0.238	0.006	0.232
2	–0.08	0.242	0.006	0.235
3	–0.86	0.241	0.004	0.237
4	–0.60	0.188	0.004	0.184
5	–0.85	0.241	0.004	0.237

Table S13 The adsorption energy, Zero-point energy (ZPE), entropic corrections (TS) at T=298 K to the free energies and (ZPE–TS) values of the structure of BL-s borophene.

BL-s-Top	ΔE_{H^*}/eV	ZPE/eV	*TS*/eV	ZPE – *TS*/eV
1	–0.20	0.227	0.009	0.218
2	–0.29	0.232	0.003	0.229
3	0.51	0.240	0.006	0.234
4	–0.20	0.228	0.009	0.219
5	–0.20	0.227	0.009	0.218
6	0.50	0.240	0.006	0.234
BL-s-Bridge	ΔE_{H^*}/eV	ZPE/eV	*TS*/eV	ZPE – *TS*/eV
1-2	–0.20	0.227	0.009	0.218
1-3	–0.20	0.227	0.009	0.218
1-4	0.17	0.227	0.004	0.222
1-6	–0.19	0.229	0.009	0.220
2-3	–0.20	0.228	0.009	0.219
3-4	–0.19	0.227	0.009	0.218
4-5	–0.28	0.232	0.003	0.229
4-6	–0.19	0.228	0.009	0.219
5-6	–0.19	0.228	0.009	0.219

Table S14 The adsorption energy, Zero-point energy (ZPE), entropic corrections (TS) at T=298 K to the free energies and (ZPE–TS) values of the structure of BL-t borophene.

BL-t-Top	ΔE_{H^*}/eV	ZPE/eV	*TS*/eV	ZPE – *TS*/eV
1	0.20	0.223	0.010	0.213
2	1.12	0.221	0.009	0.212
3	1.12	0.221	0.009	0.212
4	0.22	0.229	0.008	0.221

5	0.23	0.229	0.008	0.221

Table S15 H adsorption energies under based on the explicit solvent model (E_1), implicit solvent model (E_2), and vacuum (E_3) for BL-x borophene (x=β, i, s) catalysts at the same site.

	E_1/eV	E_2/eV	E_3/eV
BL-β borophene	–0.198	–0.174	–0.221
BL-i borophene	–0.225	–0.251	–0.238
BL-s borophene	–0.245	–0.214	–0.199

Table S16 Calculation of the ΔG_{H^*} for H adsorption in acidic media for different pH values on the structure of BL-α borophene.

BL-α-Top	PH = 0	PH = 1	PH = 2	PH = 3	PH = 4	PH = 5	PH = 6	PH = 7
1	–0.252	–0.193	–0.134	–0.075	–0.016	0.043	0.102	0.161
2	–0.253	–0.194	–0.135	–0.076	–0.017	0.042	0.101	0.160
3	0.724	0.783	0.842	0.901	0.960	1.019	1.078	1.137
4	–0.253	–0.194	–0.135	–0.076	–0.017	0.042	0.101	0.160
5	–0.253	–0.194	–0.135	–0.076	–0.017	0.042	0.101	0.160

Table S17 Calculation of the ΔG_{H^*} for H adsorption in acidic media for different pH values on the structure of BL-β borophene. The highlighted data in yellow are data with ΔG_{H^*} values within the range of –0.10 eV ~ 0.10 eV.

BL-β	PH = 0	PH = 1	PH = 2	PH = 3	PH = 4	PH = 5	PH = 6	PH = 7
m	0.502	0.561	0.620	0.679	0.738	0.797	0.856	0.915
1	–0.209	–0.150	–0.091	–0.032	0.027	0.086	0.145	0.204
2	–0.011	0.048	0.107	0.166	0.225	0.284	0.343	0.402
3	0.082	0.141	0.200	0.259	0.318	0.377	0.436	0.495
4	0.012	0.071	0.130	0.189	0.248	0.307	0.366	0.425

5	–0.033	0.026	0.085	0.144	0.203	0.262	0.321	0.380
m-1	–0.199	–0.140	–0.081	–0.022	0.037	0.096	0.155	0.214
m-2	–0.065	–0.006	0.053	0.112	0.171	0.230	0.289	0.348
m-3	0.093	0.152	0.211	0.270	0.329	0.388	0.447	0.506
m-4	0.444	0.503	0.562	0.621	0.680	0.739	0.798	0.857
m-5	0.007	0.066	0.125	0.184	0.243	0.302	0.361	0.420
m-6	0.269	0.328	0.387	0.446	0.505	0.564	0.623	0.682
1-2	–0.096	–0.037	0.022	0.081	0.140	0.199	0.258	0.317
1-3	0.301	0.360	0.419	0.478	0.537	0.596	0.655	0.714
1-4	–0.199	–0.140	–0.081	–0.022	0.037	0.096	0.155	0.214
1-5	0.269	0.328	0.387	0.446	0.505	0.564	0.623	0.682
2-3	0.082	0.141	0.200	0.259	0.318	0.377	0.436	0.495
2-4	0.400	0.459	0.518	0.577	0.636	0.695	0.754	0.813
3-3	0.154	0.213	0.272	0.331	0.390	0.449	0.508	0.567
3-4	0.082	0.141	0.200	0.259	0.318	0.377	0.436	0.495
3-5	0.082	0.141	0.200	0.259	0.318	0.377	0.436	0.495
4-3	0.174	0.233	0.292	0.351	0.410	0.469	0.528	0.587
4-4	0.012	0.071	0.130	0.189	0.248	0.307	0.366	0.425
4-5	0.012	0.071	0.130	0.189	0.248	0.307	0.366	0.425

Table S18 Calculation of the ΔG_{H^*} for H adsorption in acidic media for different pH values on the structure of BL-i borophene. The highlighted data in yellow are data with ΔG_{H^*} values within the range of –0.10 eV ~ 0.10 eV.

BL-i	PH = 0	PH = 1	PH = 2	PH = 3	PH = 4	PH = 5	PH = 6	PH = 7
1	–0.269	–0.210	–0.151	–0.092	–0.033	0.026	0.085	0.144
2	0.222	0.281	0.340	0.399	0.458	0.517	0.576	0.635
3	–0.002	0.057	0.116	0.175	0.234	0.293	0.352	0.411
4	–0.268	–0.209	–0.150	–0.091	–0.032	0.027	0.086	0.145
5	0.088	0.147	0.206	0.265	0.324	0.383	0.442	0.501

6	0.283	0.342	0.401	0.460	0.519	0.578	0.637	0.696
1-2	0.222	0.281	0.340	0.399	0.458	0.517	0.576	0.635
1-4	0.222	0.281	0.340	0.399	0.458	0.517	0.576	0.635
2-3	–0.002	0.057	0.116	0.175	0.234	0.293	0.352	0.411
2-4	–0.268	–0.209	–0.150	–0.091	–0.032	0.027	0.086	0.145
3-4	–0.268	–0.209	–0.150	–0.091	–0.032	0.027	0.086	0.145
3-5	–0.002	0.057	0.116	0.175	0.234	0.293	0.352	0.411
3-6	0.350	0.409	0.468	0.527	0.586	0.645	0.704	0.763
4-5	–0.267	–0.208	–0.149	–0.090	–0.031	0.028	0.087	0.146
4-6	–0.267	–0.208	–0.149	–0.090	–0.031	0.028	0.087	0.146
5-6	–0.267	–0.208	–0.149	–0.090	–0.031	0.028	0.087	0.146

Table S19 Calculation of the ΔG_{H^*} for H adsorption in acidic media for different pH values on the structure of BL-m borophene. The highlighted data in yellow are data with ΔG_{H^*} values within the range of –0.10 eV ~ 0.10 eV.

BL-m-Top	PH = 0	PH = 1	PH = 2	PH = 3	PH = 4	PH = 5	PH = 6	PH = 7
1	–0.370	–0.311	–0.252	–0.193	–0.134	–0.075	–0.016	0.043
2	–0.382	–0.323	–0.264	–0.205	–0.146	–0.087	–0.028	0.031
3	–0.428	–0.369	–0.310	–0.251	–0.192	–0.133	-0.074	-0.015
4	–0.327	–0.268	–0.209	–0.150	–0.091	–0.032	0.027	0.086
5	0.240	0.299	0.358	0.417	0.476	0.535	0.594	0.653
6	–0.328	–0.269	–0.210	–0.151	–0.092	–0.033	0.026	0.085
7	–0.330	–0.271	–0.212	–0.153	–0.094	–0.035	0.024	0.083
8	–0.327	–0.268	–0.209	–0.150	–0.091	–0.032	0.027	0.086

Table S20 Calculation of the ΔG_{H^*} for H adsorption in acidic media for different pH values on the structure of BL-n borophene. The highlighted data in yellow are data with ΔG_{H^*} values within the range of –0.10 eV ~ 0.10 eV.

BL-n-Top	PH = 0	PH = 1	PH = 2	PH = 3	PH = 4	PH = 5	PH = 6	PH = 7
1	0.474	0.533	0.592	0.651	0.710	0.769	0.828	0.887
2	0.155	0.214	0.273	0.332	0.391	0.450	0.509	0.568
3	–0.624	–0.565	–0.506	–0.447	–0.388	–0.329	–0.270	–0.211
4	–0.416	–0.357	–0.298	–0.239	–0.180	–0.121	–0.062	–0.003
5	–0.613	–0.554	–0.495	–0.436	–0.377	–0.318	–0.259	–0.200

Table S21 Calculation of the ΔG_{H^*} for H adsorption in acidic media for different pH values on the structure of BL-s borophene. The highlighted data in yellow are data with ΔG_{H^*} values within the range of –0.10 eV ~ 0.10 eV.

BL-s	PH = 0	PH = 1	PH = 2	PH = 3	PH = 4	PH = 5	PH = 6	PH = 7
1	0.018	0.077	0.136	0.195	0.254	0.313	0.372	0.431
2	–0.061	–0.002	0.057	0.116	0.175	0.234	0.293	0.352
3	0.740	0.799	0.858	0.917	0.976	1.035	1.094	1.153
4	0.022	0.081	0.140	0.199	0.258	0.317	0.376	0.435
5	0.019	0.078	0.137	0.196	0.255	0.314	0.373	0.432
6	0.738	0.797	0.856	0.915	0.974	1.033	1.092	1.151
1-2	0.018	0.077	0.136	0.195	0.254	0.313	0.372	0.431
1-3	0.018	0.077	0.136	0.195	0.254	0.313	0.372	0.431
1-4	0.392	0.451	0.510	0.569	0.628	0.687	0.746	0.805
1-6	0.030	0.089	0.148	0.207	0.266	0.325	0.384	0.443
2-3	0.019	0.078	0.137	0.196	0.255	0.314	0.373	0.432
3-4	0.028	0.087	0.146	0.205	0.264	0.323	0.382	0.441
4-5	–0.051	0.008	0.067	0.126	0.185	0.244	0.303	0.362
4-6	0.022	0.081	0.140	0.199	0.258	0.317	0.376	0.435
5-6	0.023	0.082	0.141	0.200	0.259	0.318	0.377	0.436

Table S22 Calculation of the ΔG_{H^*} for H adsorption in acidic media for different pH values on the structure of BL-t borophene. The highlighted data in yellow are data with ΔG_{H^*} values within the range of –0.10 eV ~ 0.10 eV.

BL-α-Top	PH = 0	PH = 1	PH = 2	PH = 3	PH = 4	PH = 5	PH = 6	PH = 7
1	0.416	0.475	0.534	0.593	0.652	0.711	0.770	0.829
2	1.331	1.390	1.449	1.508	1.567	1.626	1.685	1.744
3	1.331	1.390	1.449	1.508	1.567	1.626	1.685	1.744
4	0.445	0.504	0.563	0.622	0.681	0.740	0.799	0.858
5	0.446	0.505	0.564	0.623	0.682	0.741	0.800	0.859

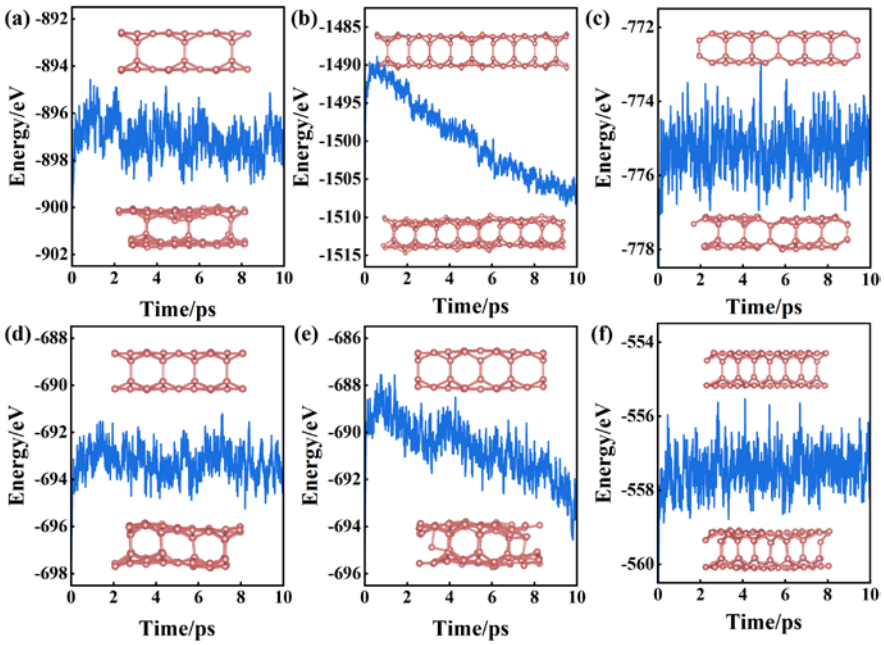


Fig. S1 Evolution of the total energy of AIMD simulation for (a) BL-α borophene, (b) BL-l borophene, (c) BL-m borophene, (d) BL-n borophene, (e) BL-o borophene and (f) BL-t borophene at 300 K. The inset are snapshot structures of BL-x borophene (x=α, l, m, n, o, t) at 10 ps.

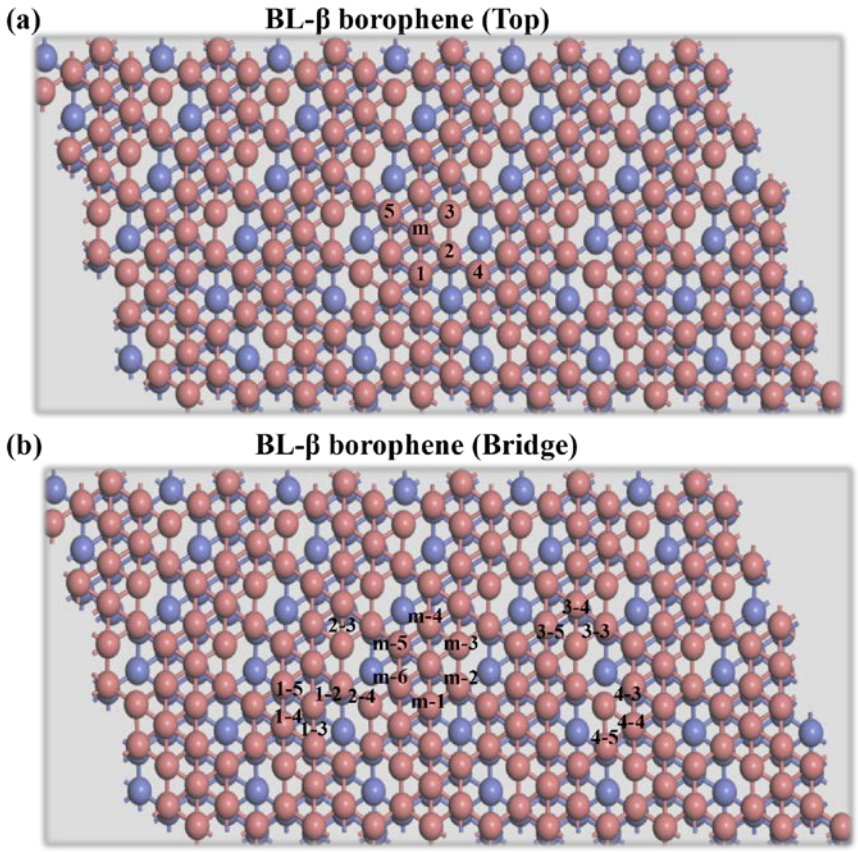


Fig. S2 Division of various possible adsorption sites of BL-β borophene. (a) Top site, (b) Bridge site. The boron atoms on the top and bottom layers are labeled with pink and light purple, respectively.

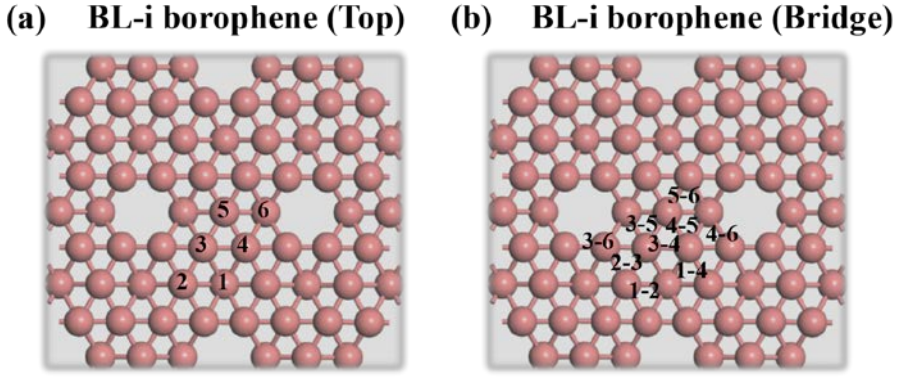


Fig. S3 Division of various possible adsorption sites of BL-i borophene. (a) Top site, (b) Bridge site. The boron atoms on the top and bottom layers are labeled with pink and light purple, respectively.

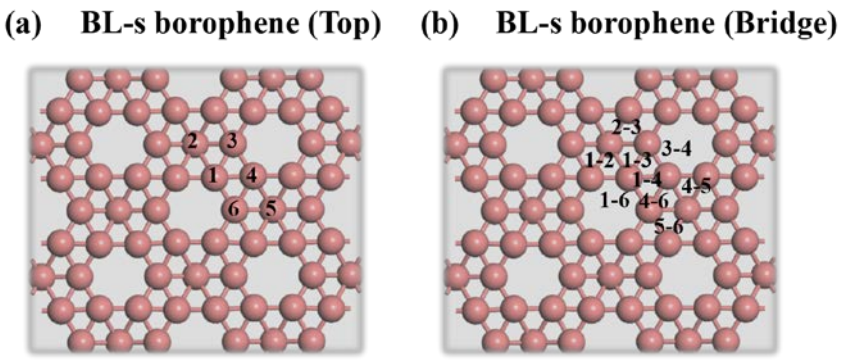


Fig. S4 Division of various possible adsorption sites of BL-s borophene. (a) Top site, (b) Bridge site. The boron atoms on the top and bottom layers are labeled with pink and light purple, respectively.

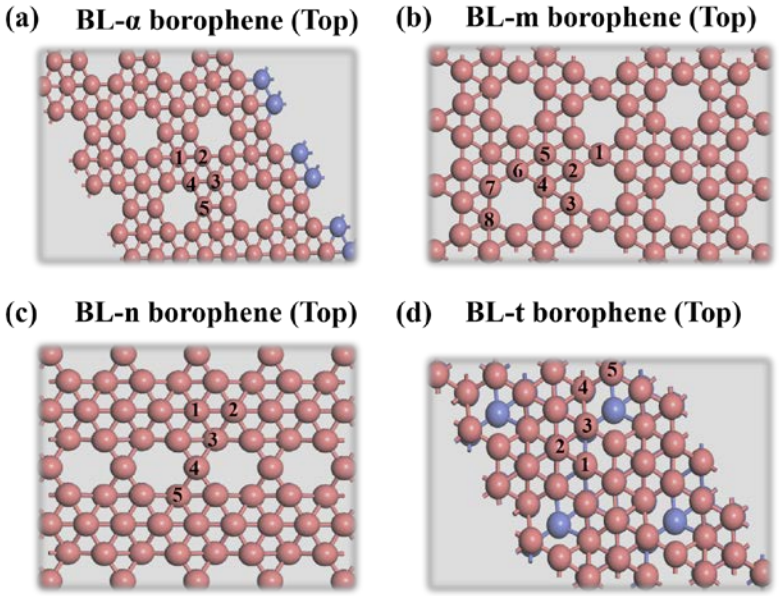


Fig. S5 Division of various possible adsorption sites of (a) BL-α borophene, (b) BL-m borophene, (c) BL-n borophene and BL-t borophene. The boron atoms on the top and bottom layers are labeled with pink and light purple, respectively.

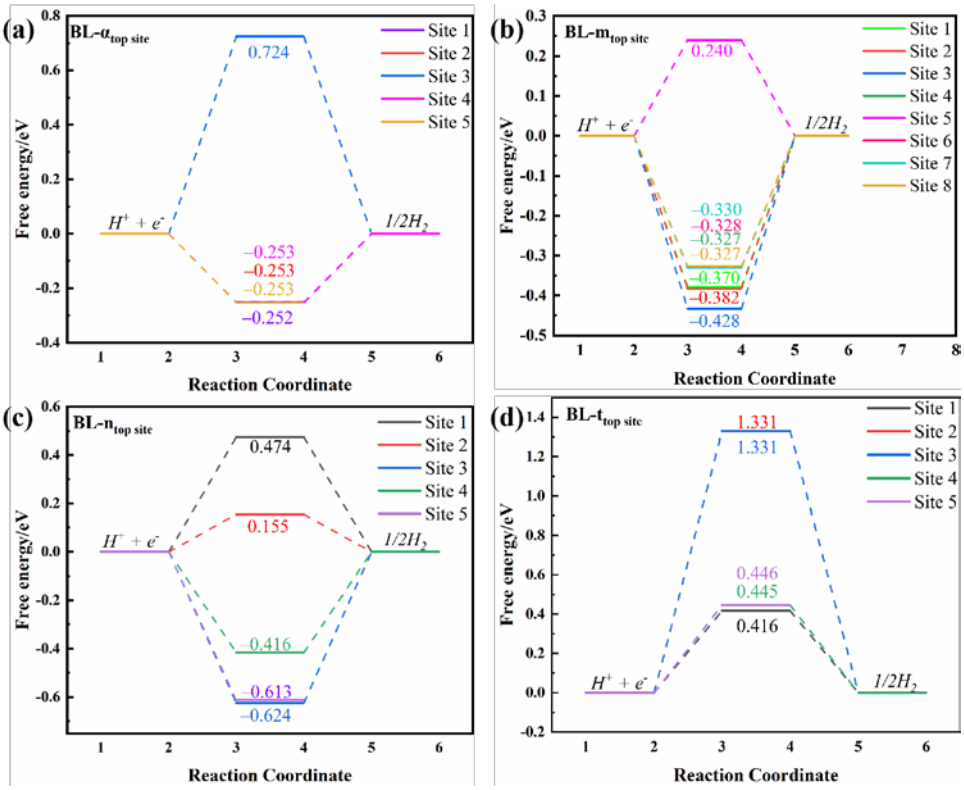
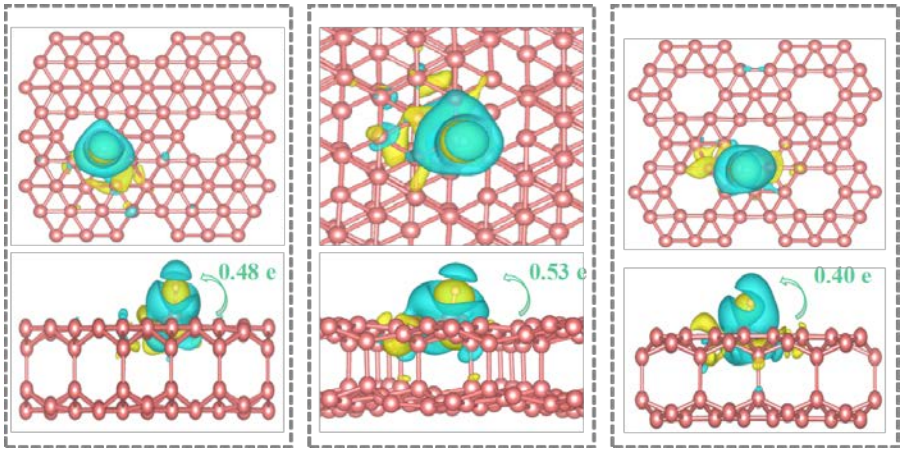


Fig. S6 Free energy diagram of hydrogen evolution over (a) BL-α borophene, (b) BL-m borophene, (c) BL-n borophene and (d) BL-t borophene catalysts at zero potential and pH = 0.



(a) **(b)** **(c)**

Fig. S7 The Charge density difference illustrations of H adsorbed over BL-x borophene (x=β, i, s), (a) BL-i borophene at top site 3, (b) BL-β borophene at bridge site (m-5) and (c) BL-s borophene at top site 1, respectively. Here, yellow and blue areas represent charge accumulation and deficiency, respectively.

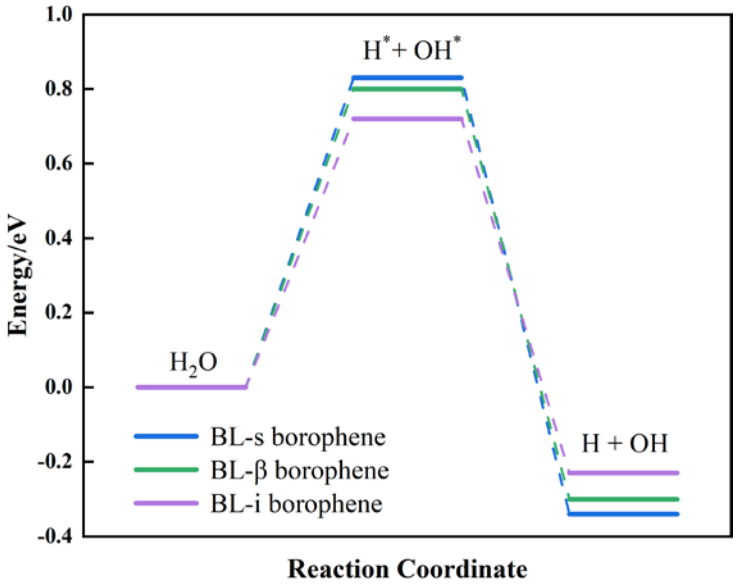


Fig. S8 Barriers of water molecule dissociation on the surface of BL-x borophene (x=β, i, s), respectively.

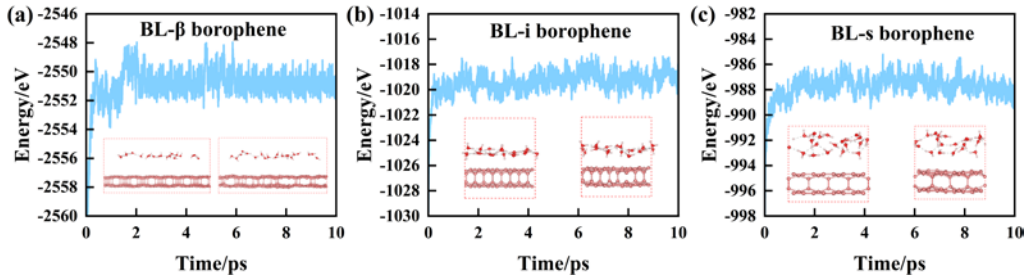


Fig. S9 Evolution of the total energy of AIMD simulation for (a) BL-β borophene, (b) BL-i borophene and (c) BL-s borophene catalysts at 300 K in a water environment. The inset are snapshot structures of BL-x borophene (x=β, i, s) catalysts at 10 ps.

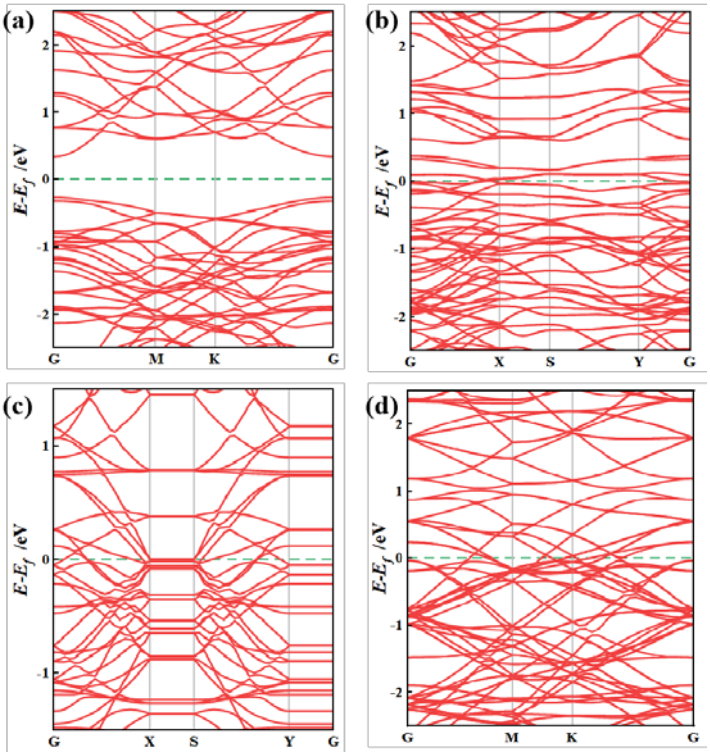


Fig. S10 Band structures of the (a) BL-t borophene, (b) BL-m borophene, (c) BL-n borophene and (d) BL-α borophene catalysts.

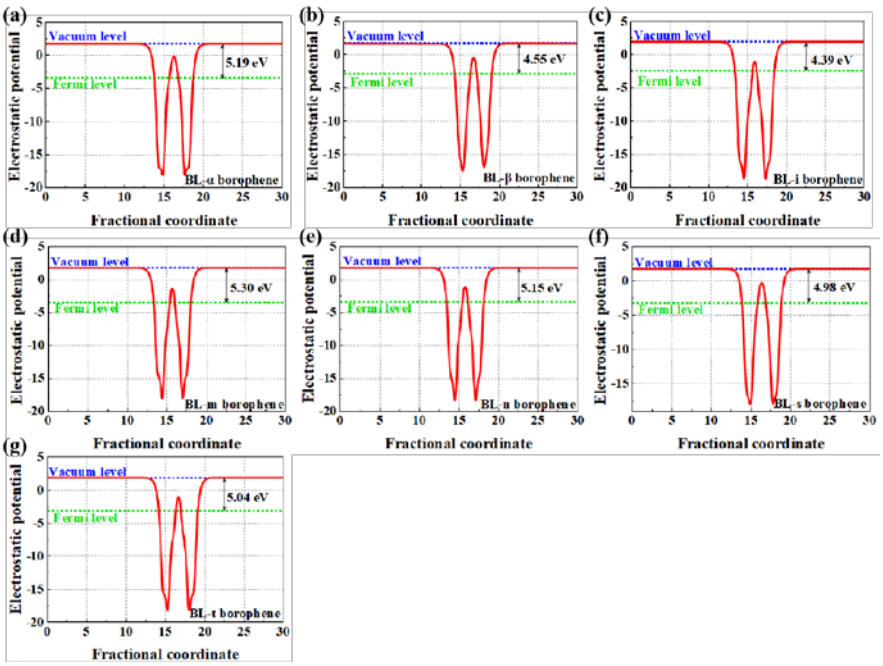


Fig. S11 Electrostatic potentials of (a) BL-α borophene, (b) BL-β borophene, (c) BL-i borophene, (d) BL-m borophene, (e) BL-n borophene, (f) BL-s borophene, (g) BL-t borophene catalysts.

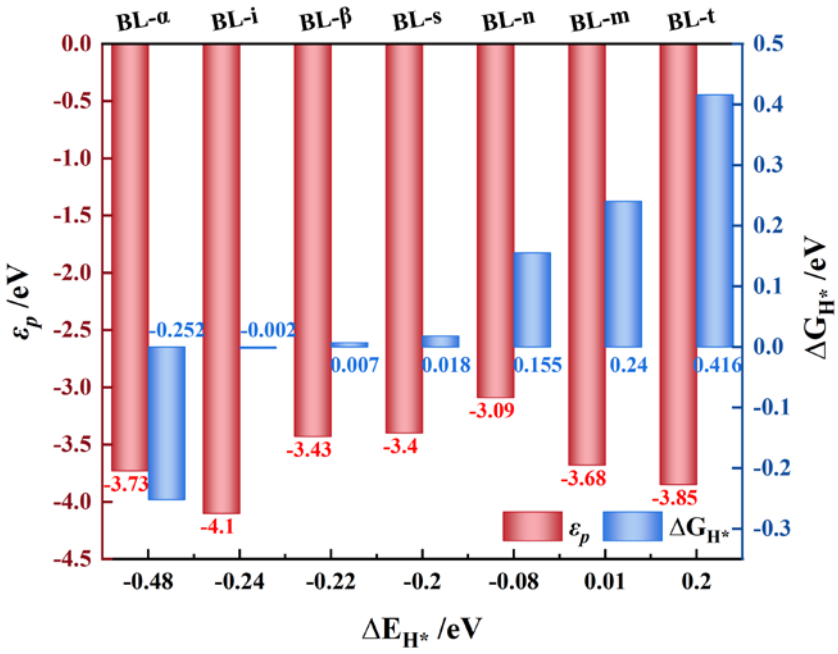


Fig. S12 The most advantageous *p*-band center (ε_p) and free energy ΔG_{H^*} for the BL-x borophene (x=α, β, i, m, n, s, t) adsorption performance.