Supplementary Information

Promising transition metal decorated borophene catalyst for water splitting

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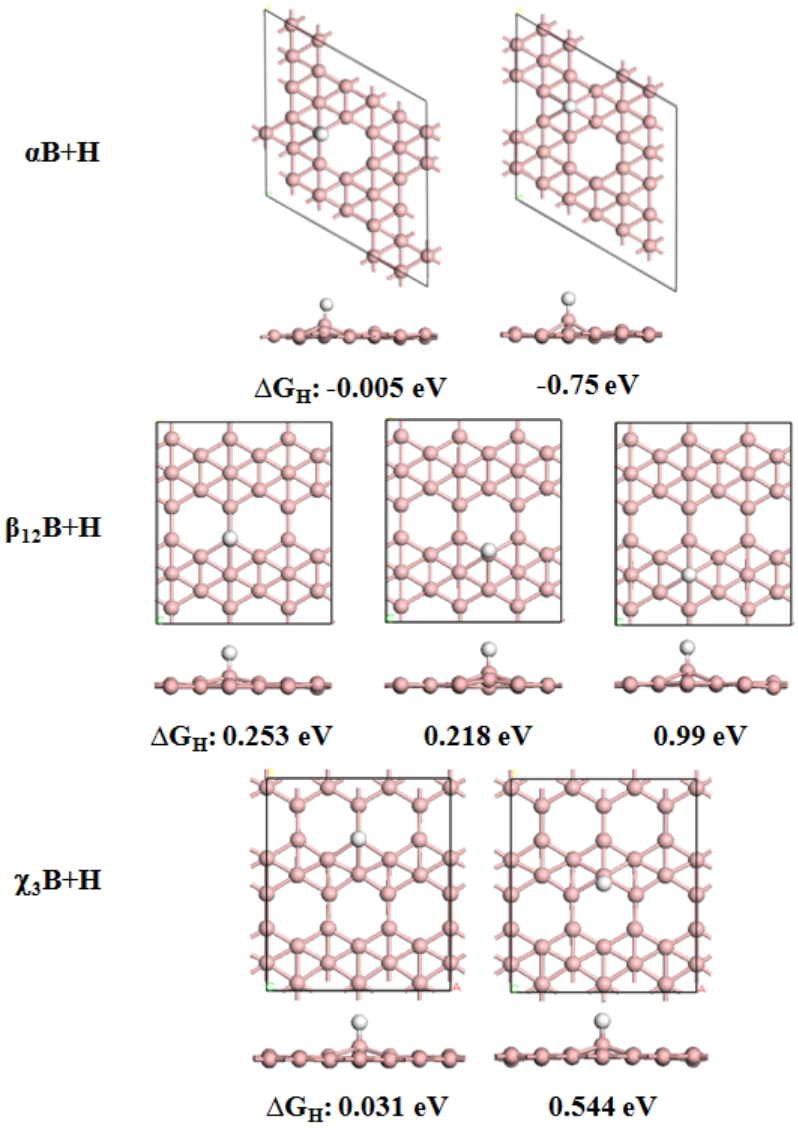

Fig. S1 The top and side views of H adsorption structures of αB, β_{12}B and χ_3B; the corresponding H adsorption free energies are listed below the structures. The pink ball represents B atom and white ball represents H atom.

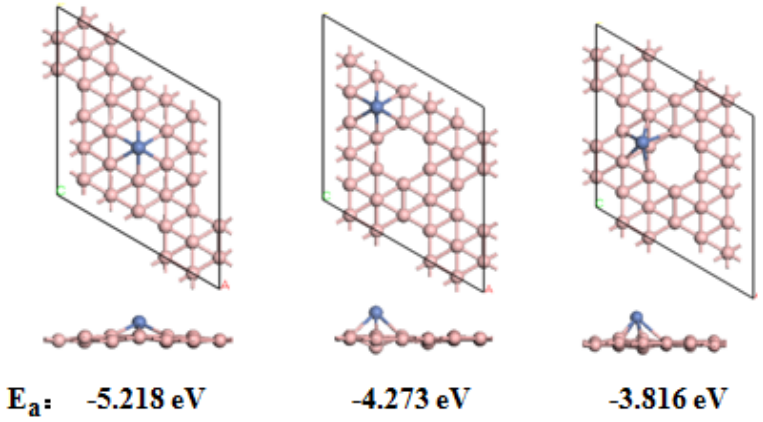

Fig. S2 Ni adsorption sites and adsorption energies on αB.

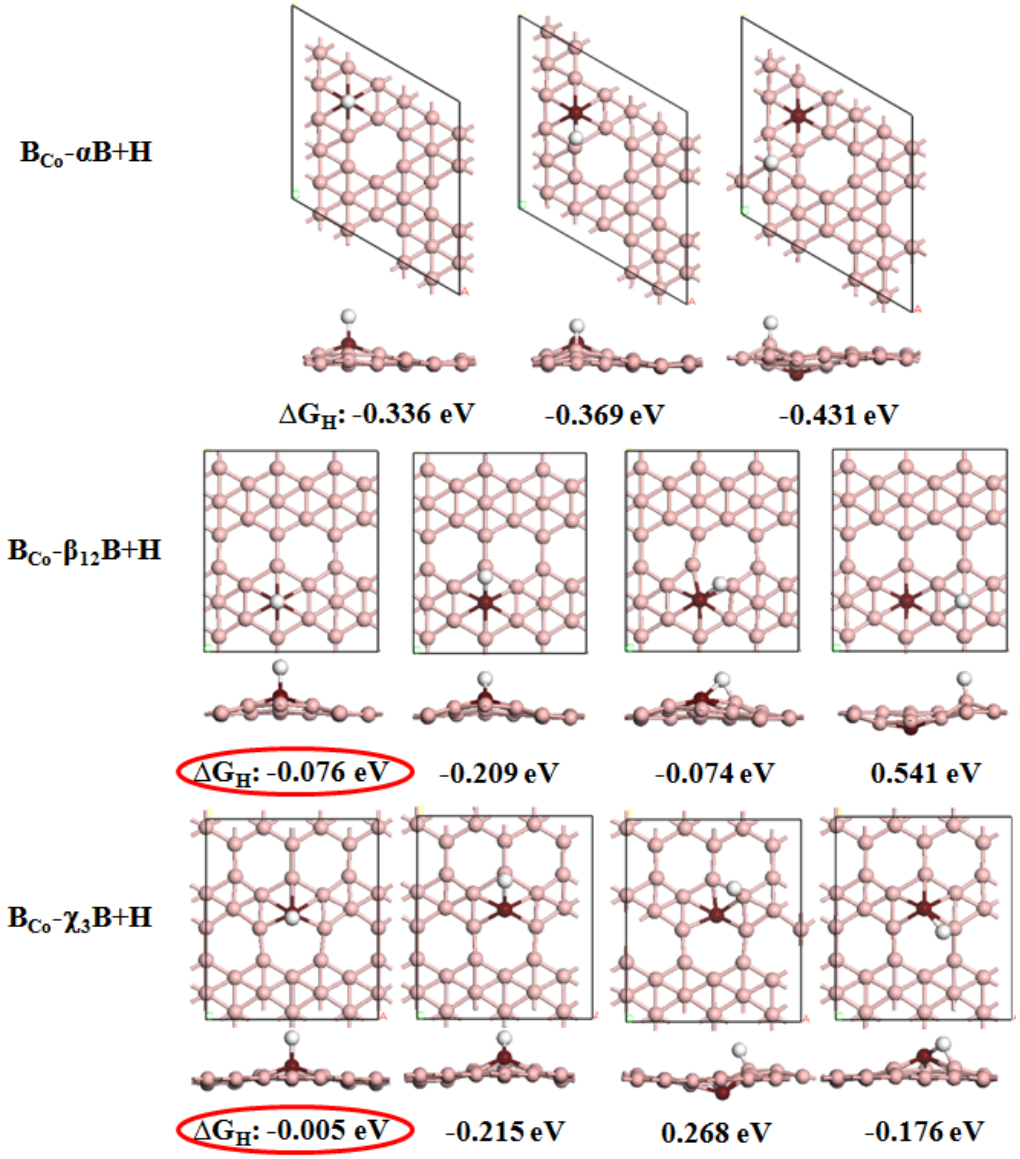

Fig. S3 The top and side views of H adsorption structures of B_{Co}- doped αB, B_{Co}-doped β_{12}B and B_{Co}- doped χ_3B; the corresponding H adsorption free energies are listed below the structures. Here, the pink, brown and white balls represent B, Co and H atoms, respectively.

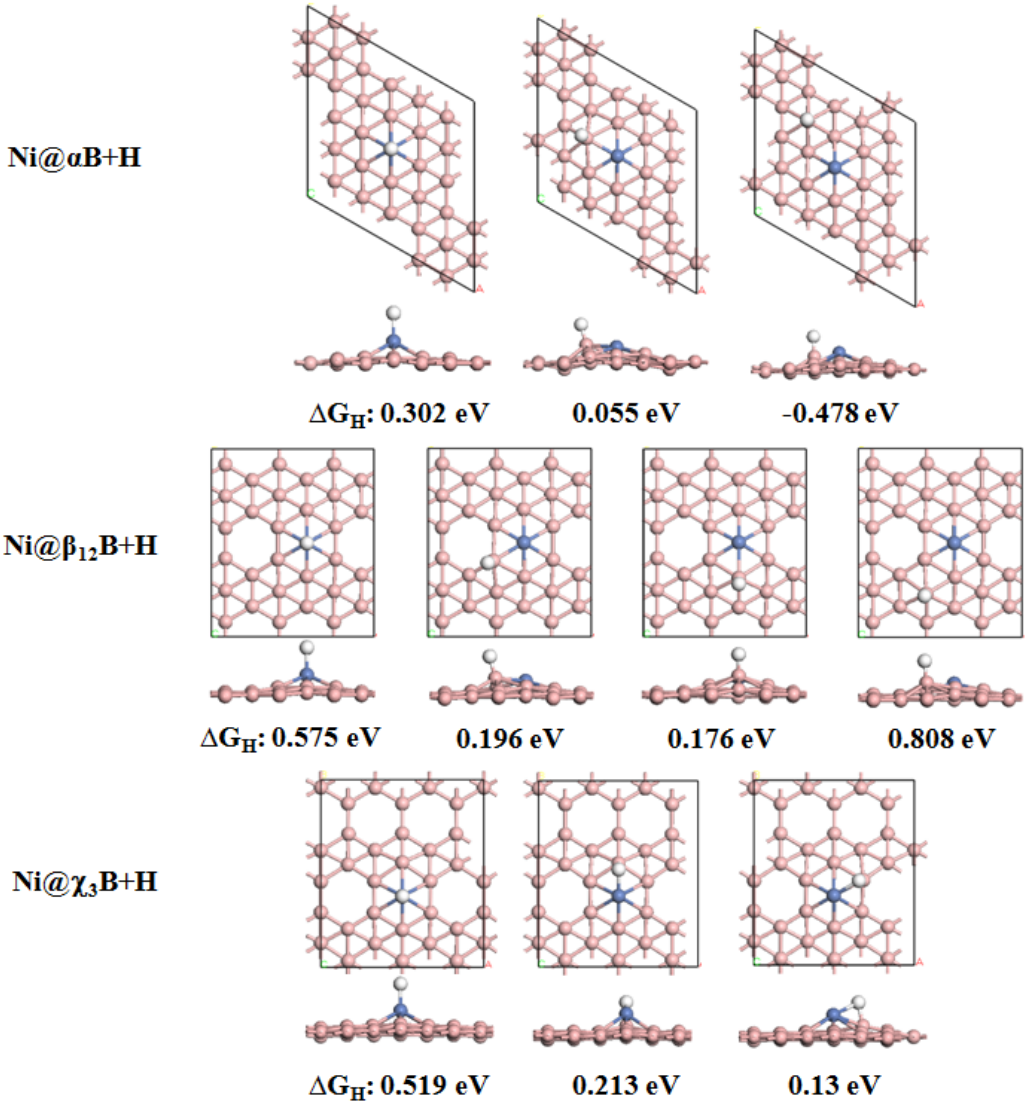

Fig. S4 The top and side views of H adsorption structures of Ni- doped αB, Ni- doped β_{12}B and Ni- doped χ_3B; the corresponding H adsorption free energies are listed below the structures. Here, the pink, blue and white balls represent B, Ni and H atoms, respectively.

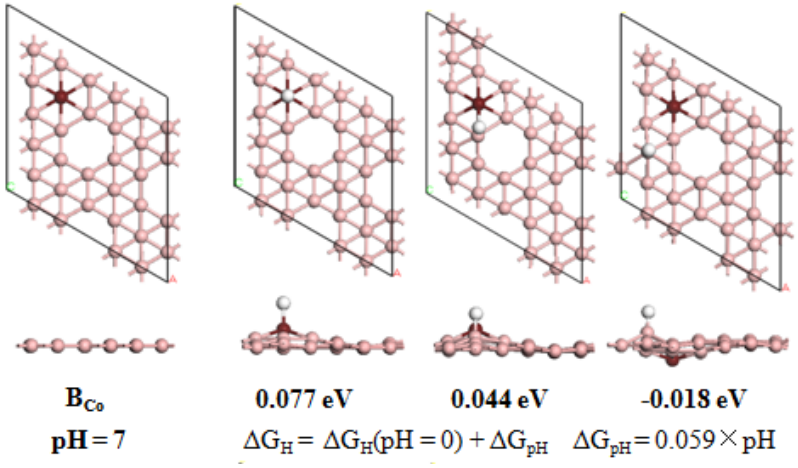

Fig. S5 H adsorption sites and free energies on B_{Co}- doped αB when pH = 7.

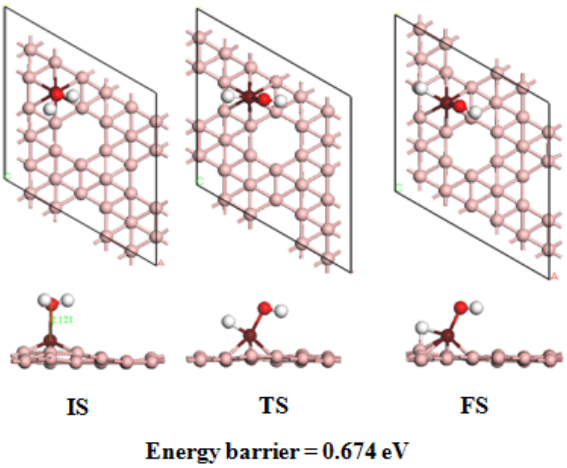

Fig. S6 Initial state (IS), transition state (TS), final state (FS) for water dissociation on B_{Co}- doped αB. Here, the pink, brown, red and white balls represent B, Co, O and H atoms, respectively.

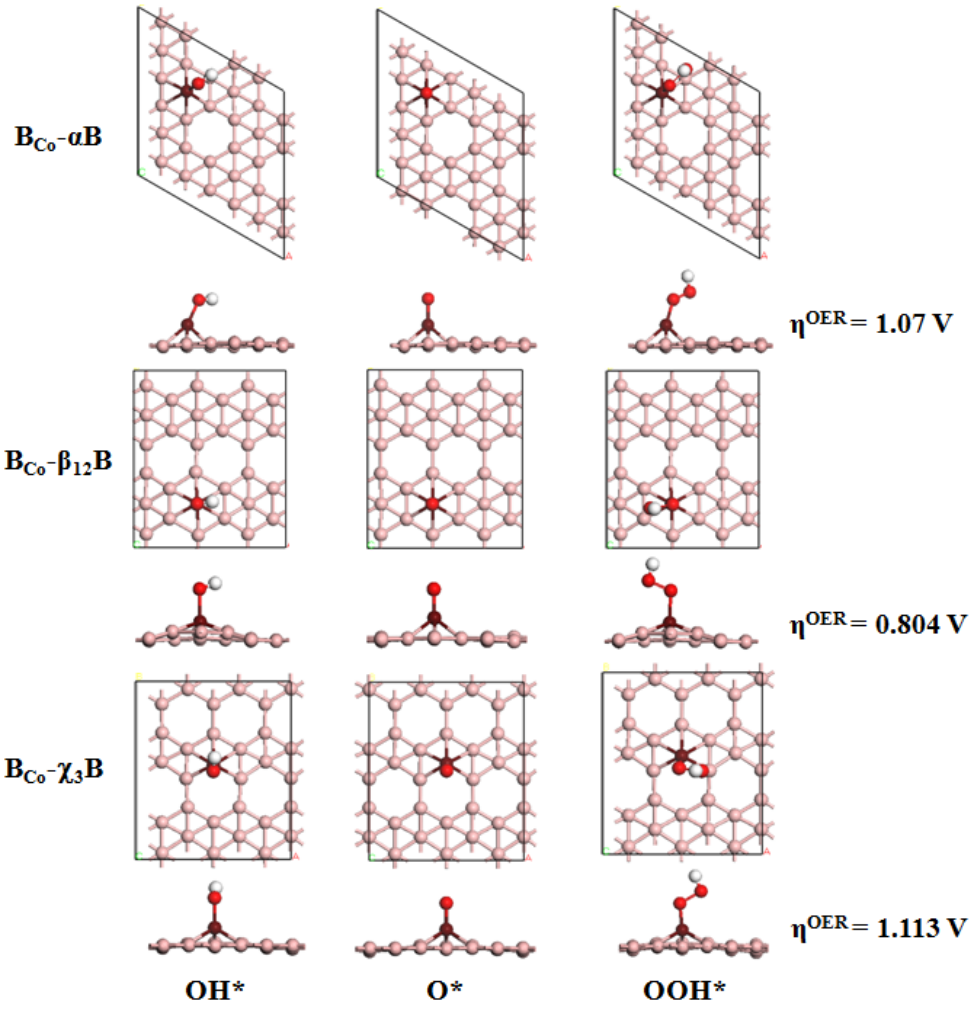

Fig. S7 The top and side views of structures of the adsorbed intermediates (OH*, O* and OOH*) on B_{Co}- doped borophenes. The overpotentials are listed on the right side of the structures. Here, the pink, brown, red and white balls represent B, Co, O and H atoms, respectively.

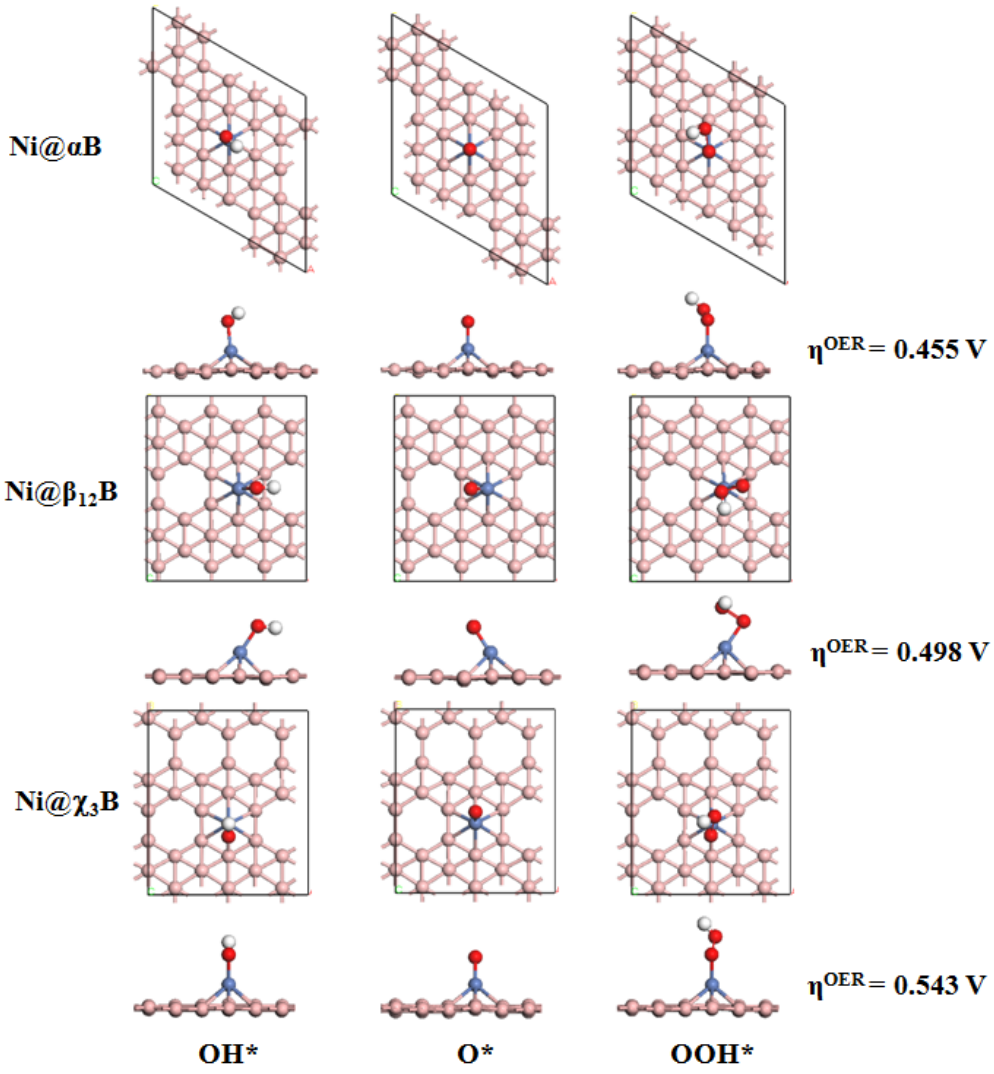

Fig. S8 The top and side views of structures of the adsorbed intermediates (OH*, O* and OOH*) on Ni- doped borophenes. The overpotentials are listed on the right side of the structures. Here, the pink, blue, red and white balls represent B, Ni, O and H atoms, respectively.

Table. S1 The reaction Gibbs free energy (ΔG_1, ΔG_2, ΔG_3 and ΔG_4) of four elementary steps and overpotential (η^{OER}) for OER.

	ΔG_1/eV	ΔG_2/eV	ΔG_3/eV	ΔG_4/eV	η^{OER}/V
B_{Co}-αB	-0.278	0.82	2.3	2.078	1.07
B_{Co}-β_{12}B	1.126	1.068	2.034	0.692	0.804
B_{Co}-χ_3B	0.299	0.762	2.343	1.516	1.113
Ni@αB	0.627	1.685	1.537	1.071	0.455
Ni@β_{12}B	1.001	1.492	1.728	0.699	0.498
Ni@χ_3B	0.583	1.434	1.773	1.13	0.543

Table. S2 The adsorption energies of intermediates (OH*, O* and OOH*) on B_{Co}- and Ni- doped borophenes in OER process.

	***OH**	***O**	***OOH**
B_{Co}-αB	-0.664	0.492	2.392
B_{Co}-β_{12}B	0.746	2.14	3.772
B_{Co}-χ_3B	-0.067	1.004	2.944
Ni@αB	0.265	2.271	3.401
Ni@β_{12}B	0.621	2.45	3.743
Ni@χ_3B	0.201	1.97	3.328