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

Supporting Information

HER catalytic activity and regulation of transition metal atom anchored BC_3 monolayer: A first−principles study

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Table S1 Hydrogen adsorption energy (in eV) at different adsorption sites in the TM@BC_3 system. Slashes indicate non-adsorption cases.

	Ti	Fe	Cu	Zn	Mo	Ag	Au
C1	0.48	0.11	0.19	0.20	0.38	0.15	0.14
C2	0.72	0.16	0.56	0.55	−0.04	0.55	0.44
C3	0.16	−0.22	−0.10	−0.20	−0.25	−0.05	−0.04
C4	0.68	0.58	0.57	0.57	0.55	0.58	0.60
C5	/	0.75	0.68	/	/	0.69	0.68
M	−0.05	0.15	/	−0.38	−0.28	0.22	−0.25
B1	0.11	0.56	0.26	0.26	0.06	0.23	0.21
B2	−1.23	−0.43	−0.81	−0.77	−0.79	−0.52	−0.32

Table S2 Hydrogen adsorption energy (in eV) at different adsorption sites in the O/TM@BC_3 system. Slashes indicate non-adsorption cases.

	Ti	Cu	Zn	Mo
C1	0.57	−0.47	0.18	0.20
C2	0.93	0.52	0.83	0.38
C3	0.60	−0.53	0.00	−0.87
C4	0.50	0.00	0.38	0.58
C5	0.68	0.50	0.68	0.86
M	0.81	/	0.70	−0.62
B1	0.90	0.54	0.71	0.81
B2	1.68	/	1.73	−0.63
O	0.48	−1.19	−0.25	−1.08