The performance of adsorption, dissociation and diffusion mechanism of hydrogen on the Ti-doped ZrCo(110) surface

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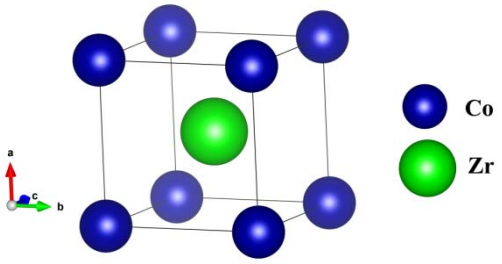

Fig. S1 Crystal structure of ZrCo alloys

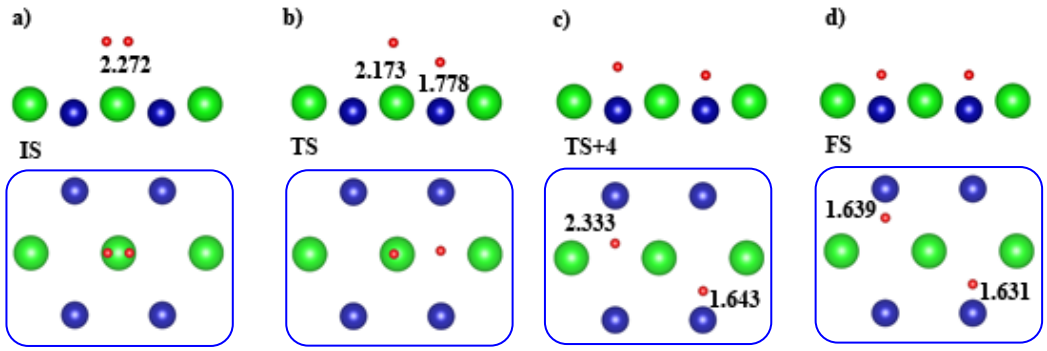

Fig. S2 a) initial state, b) transition state, c) transition state+4 d) final state Points, calculated states from H_2 dissociation on the pure surface.

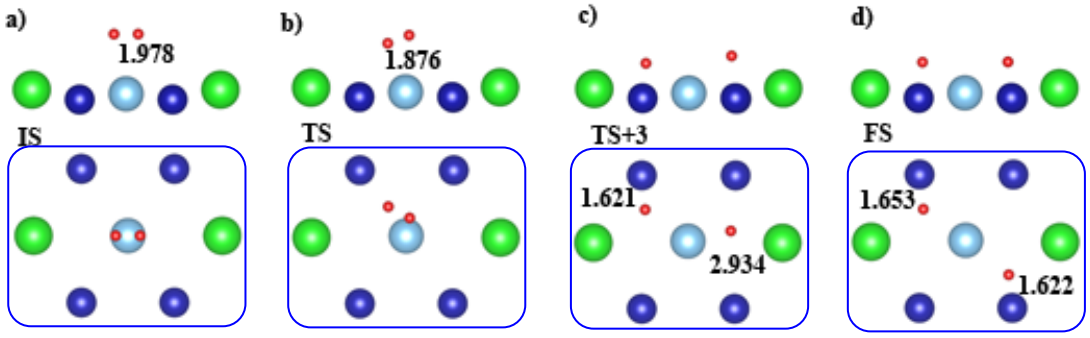

Fig. S3 a) initial state, b) transition state, c) transition state+3 d) final state Points, calculated states from H_2 dissociation on the doped surfaces.

Table S1 The direct coordinates of ZrCo(110) and Ti-ZrCo(110) surface atoms in the z direction. d_{12} and d_{23} are the change in layer spacing between the first and second layers and between the second and third layers, respectively

Layer (from top layer)	ZrCo(110) surface			Ti-ZrCo(110) surface		
	Before relaxation	After relaxation	Δ	Before relaxation	After relaxation	Δ
1^{st}(Co)	11.245	10.984	-0.261	11.245	10.990	-0.255
1^{st}(Zr)	11.245	11.295	0.050	11.245	11.296	0.051
1^{st}(Ti)	-	-	-	11.245	11.077	-0.168
2^{nd}(Zr)	8.996	9.002	0.006	8.996	9.013	0.017
2^{nd}(Co)	8.996	9.153	0.157	8.996	9.179	0.183
3^{rd}(Co)	6.747	6.680	-0.067	6.747	6.673	-0.074
3^{rd}(Zr)	6.747	6.755	0.008	6.747	6.766	0.019
d_{12}(Co-Zr)	2.249	1.982	-13.50%	2.249	1.977	-13.77%
d_{12}(Zr-Co)	2.249	2.142	-5.00%	2.249	2.117	-6.25%
d_{12}(Ti-Zr)	-	-	-	2.249	2.064	-8.97%
d_{12}(Ti-Co)	-	-	-	2.249	1.898	-18.49%
d_{23}(Zr-Co)	2.249	2.322	3.14%	2.249	2.340	3.90%
d_{23}(Co-Zr)	2.249	2.398	6.21%	2.249	2.413	6.81%

Table S2 Adsorption energy(E_{ads}) and the distance of H from the surface after H atom adsorption on ZrCo(110).

Adsorption site	E_{ads}/H(eV)	the distance of H from the surface(Å)
B1	-3.869	1.272
B2	-3.750	1.405
H1	-4.083	0.959
T1	-3.703	1.602
T2	-3.012	2.096

Table S3 Adsorption energy (E_{ads}) and the distance of H_2 from the surface after H_2 adsorption on ZrCo(110).

Adsorption site		E_{ads}/H (eV)	the distance of H_2 from the surface (Å)
B1	-a	0.285	2.000
	-b	0.0004	4.080
	-c	-0.018	3.098
B2	-a	-1.496	-

	-b	-0.007	3.861
	-c	-0.014	2.822
H1	-a	-0.006	3.885
	-b	-1.497	-
T1	-a	-1.412	-
	-b	-0.003	3.945
	-c	-0.022	3.586
T2	-a	-0.214	2.312
	-b	-0.246	2.272
	-c	-0.006	3.084

*Table S4 The adsorption energy (E_{ads}) of H atom adsorption on the Fe-doped ZrCo(110).

Adsorption site	E_{ads} (eV)
B4(CoFe)	-3.926
H1(ZrZrFe)	-4.246
T2(Zr)	-2.981

*'B' refers to 'bridge site', 'H' refers to 'hollow site', 'T refers to 'top site', and the atoms that make up the corresponding highly symmetric site are enclosed in parentheses, the same below.

Table S5 The adsorption energy (E_{ads}) of H atom adsorption on the Sc-doped ZrCo(110).

Adsorption site	E_{ads}
B1(ZrSc)	-3.684
B3(CoCo)	-3.874
H1(ZrCoSc)	-4.113
H2(CoCoSc)	-4.114
T3(Sc)	-2.676

Table S6 The adsorption energy (E_{ads}) of H atom adsorption on the Ni-doped ZrCo(110).

Adsorption site	E_{ads}
B2(ZrZr)	-3.829
B4(CoNi)	-3.810
H1(ZrZrNi)	-3.952

Table S7 The adsorption energy (E_{ads}) of H atom adsorption on the Cu-doped ZrCo(110).

Adsorption site	E_{ads}
B4(CoCu)	-3.719
H1(ZrZrCu)	-4.015
T1(Co)	-3.646
T2(Zr)	-3.067
T3(Cu)	-3.284

Table S8 The adsorption energy (E_{ads}) of H atom adsorption on the V-doped ZrCo(110).

Adsorption site	E_{ads}
B4(CoV)	-4.062
H1(ZrZrV)	-4.466

H2(ZrCoV)	-4.463
T1(Co)	-3.663
T3(V)	-3.705

Table S9 The adsorption energy (E_{ads}) of H atom adsorption on the Pt-doped ZrCo(110).

Adsorption site	E_{ads}
B2(ZrZr)	-3.651
B4(CoPt)	-3.568
H1(ZrZrPt)	-3.676
T3(Pt)	-3.347

Table S10 The adsorption energy (E_{ads}) of H atom adsorption on the Rh-doped ZrCo(110).

Adsorption site	E_{ads}
B2(ZrZr)	-3.643
B4(CoRh)	-3.776
H1(ZrZrRh)	-3.938
T1(Co)	-3.683
T3(Rh)	-3.494