Supporting information for

Effect of metal matrix M (M=Co, Ni, Cu) on the water dissociation performance of oxophilic Cr from density functional theory

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Table S1 ΔE_{H_2O}, ΔE_H, ΔE_{OH}, ΔE_O on active sites of Cr, M (Co, Ni, Cu), and Cr-M surface.

Sample	Adsorption energy	Site [a/1]	Site [b/2]	Site [c/3]	Site [d/4]
Cr	ΔE_{H_2O}	-1.44	-	**-1.58**	-
	ΔE_H	-	**-1.59**	-	-
	ΔE_{OH}	-	**-5.50**	-	-
	ΔE_O	-3.82	**-5.23**	-	-
Co	ΔE_{H_2O}	**-0.56**	-	-	-0.51
	ΔE_H	-	**-0.67**	-0.65	-
	ΔE_{OH}	-	-3.70	**-3.75**	-
	ΔE_O	-	-2.86	**-2.91**	-
Cr-Co	ΔE_{H_2O}	**-0.95**	-	-	-
	ΔE_H	-	**-0.66**	-0.63	-
	ΔE_{OH}	-3.55	-4.11	**-4.15**	-
	ΔE_O	-2.84	-3.48	**-3.58**	-
Ni	ΔE_{H_2O}	**-0.59**	-	-	-
	ΔE_H	-	**-0.65**	-0.64	-
	ΔE_{OH}	-	**-3.47**	-3.35	-
	ΔE_O	-	**-2.51**	-2.39	-
Cr-Ni	ΔE_{H_2O}	**-1.07**	-	-	-
	ΔE_H	-	**-0.73**	-0.68	-

	ΔE_{OH}	-3.64	**-3.93**	-3.81	-
	ΔE_{O}	-2.94	**-3.30**	-3.26	-
Cu	ΔE_{H_2O}	**-0.40**	-	-	-
	ΔE_{H}	-	**-0.29**	-0.28	-
	ΔE_{OH}	-	**-3.07**	-3.01	-
	ΔE_{O}	-	**-1.79**	-1.69	-
Cr-Cu	ΔE_{H_2O}	**-0.89**	-	-	-
	ΔE_{H}	0.23	**-0.44**	-0.43	-
	ΔE_{OH}	-3.56	**-3.66**	-3.61	-
	ΔE_{O}	-2.71	**-2.89**	-2.81	-

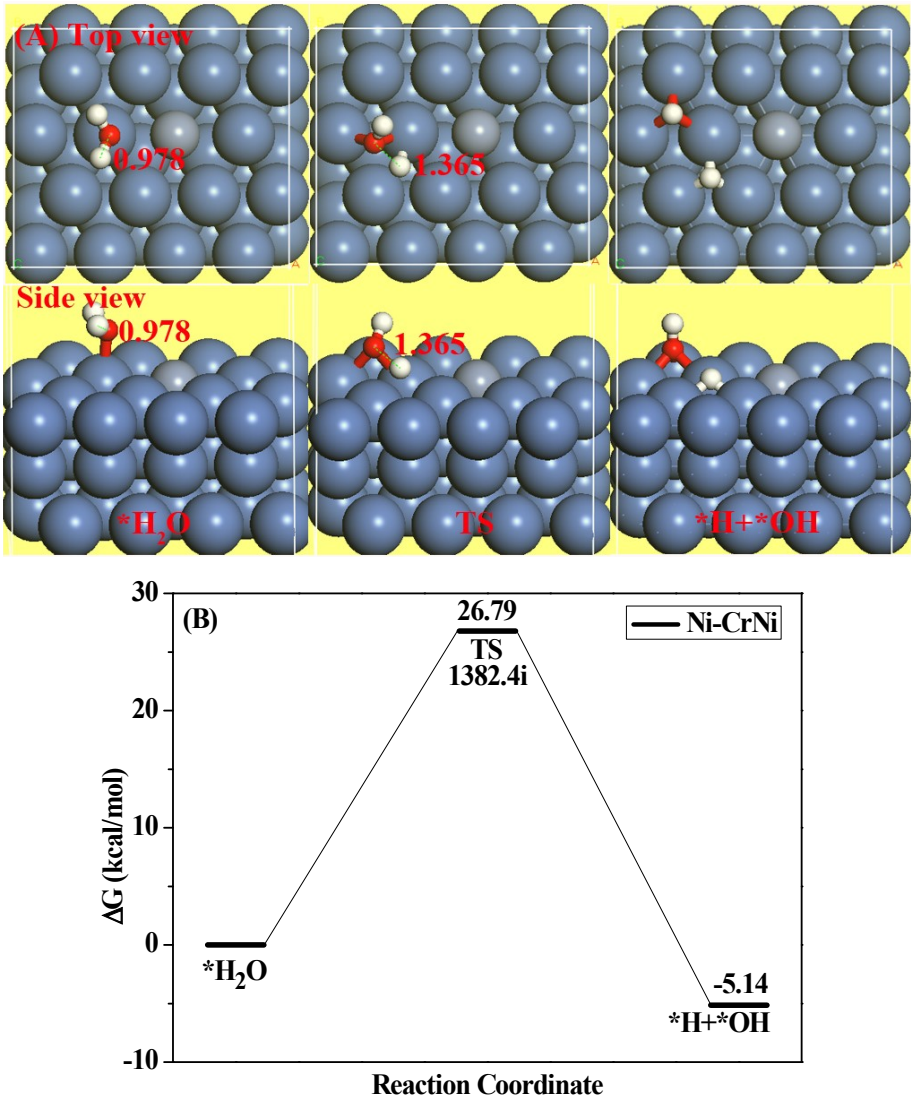

Fig. S1 (A) Optimized geometries of initial state, transition state, and final state in H_2O dissociation step on Ni adjacent to Cr in Cr-Ni (the unit of bond length is Å, the gray-blue, gray, white, and red balls represent Ni, Cr, H, and O atom, respectively); (B) Potential energy diagram for H_2O dissociation pathway on Ni adjacent to Cr in Cr-Ni.

Table S2 ΔG_H (eV) on active sites of Cr, M (Co, Ni, Cu), and Cr-M surface.

Sample	Site [a/1]	Site [b/2]	Site [c/3]	Site [d/4]
Cr	-	-1.34	-	-
Co	-	-0.43	-0.42	-
Cr-Co	-	-0.43	-0.40	-
Ni	-	-0.41	-0.40	-
Cr-Ni	-	-0.49	-0.44	-
Cu	-	-0.05	-0.05	-
Cr-Cu	0.39	-0.20	-0.19	-

Table S3 HER performance on reported transition metal catalysts in alkaline electrolyte

Catalyst	Current density (-*j*, mA cm^{-2})	-η at corresponding *j*(mV)	Tafel slope (mV dec^{-1})
Cu [21]	8	575~580	143
Ni [22]	10	322	164
Co [38]	10	~250	161
Cr-Ni [22]	10	203	124
Cr [22]	0.1	~500	-