Electronic Supplementary Information

Boosting the Hydrogen Evolution Reaction Activity of Ru in Alkaline and Neutral Media by Accelerating Water Dissociation

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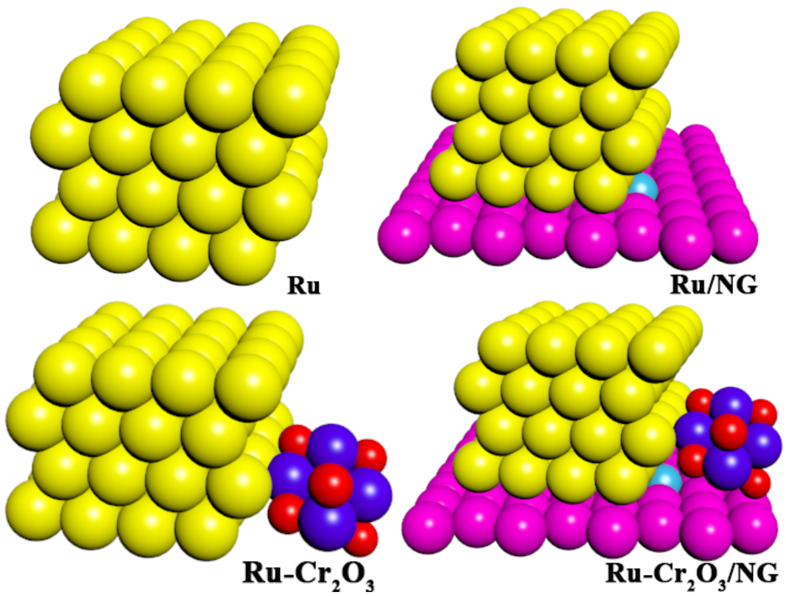

Fig. S1 Surface configuration of the four different catalysts used for the calculation

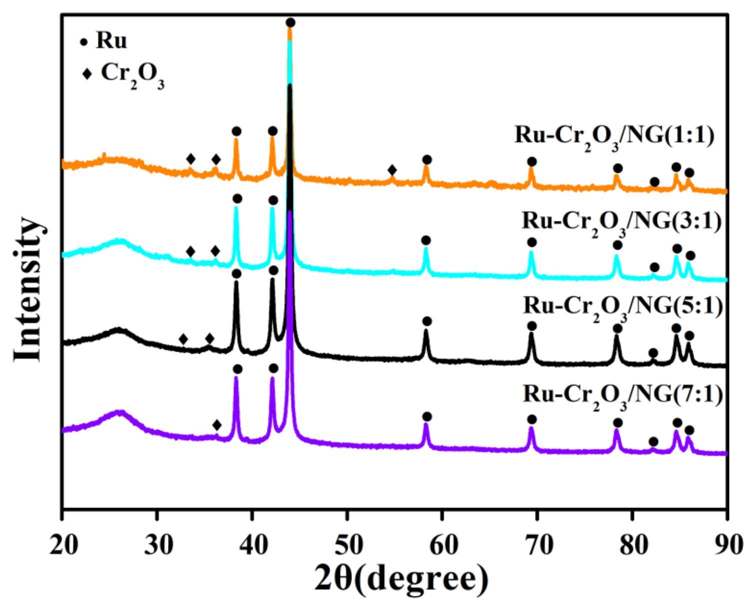

Fig. S2 XRD pattern of the Ru and Cr_2O_3 with different molar ratios in Ru-Cr_2O_3/NG.

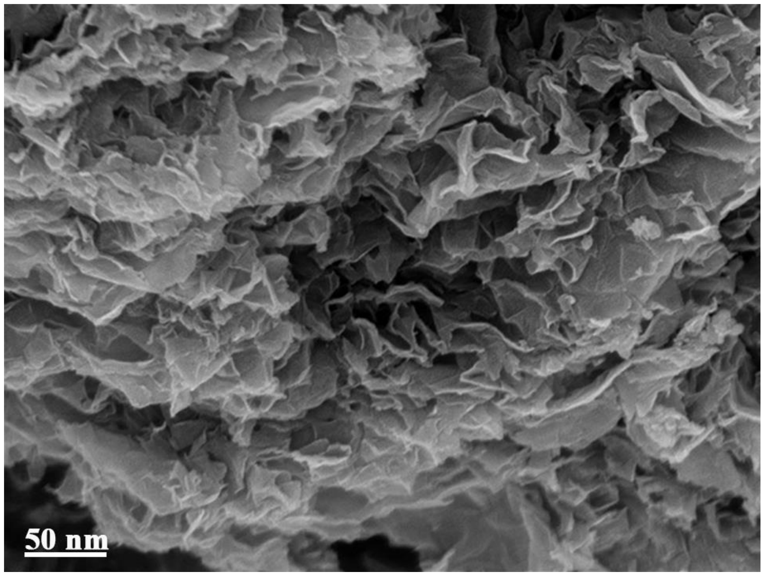

Fig. S3 SEM image of Ru-Cr_2O_3/NG.

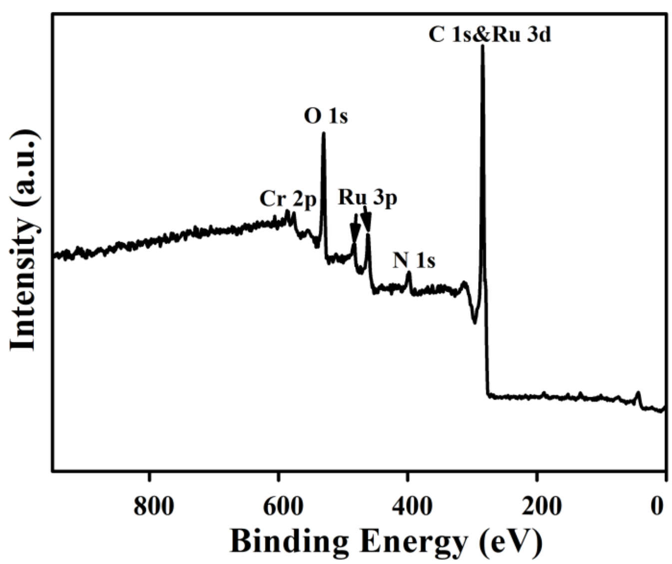

Fig. S4 XPS survey of Ru-Cr_2O_3/NG.

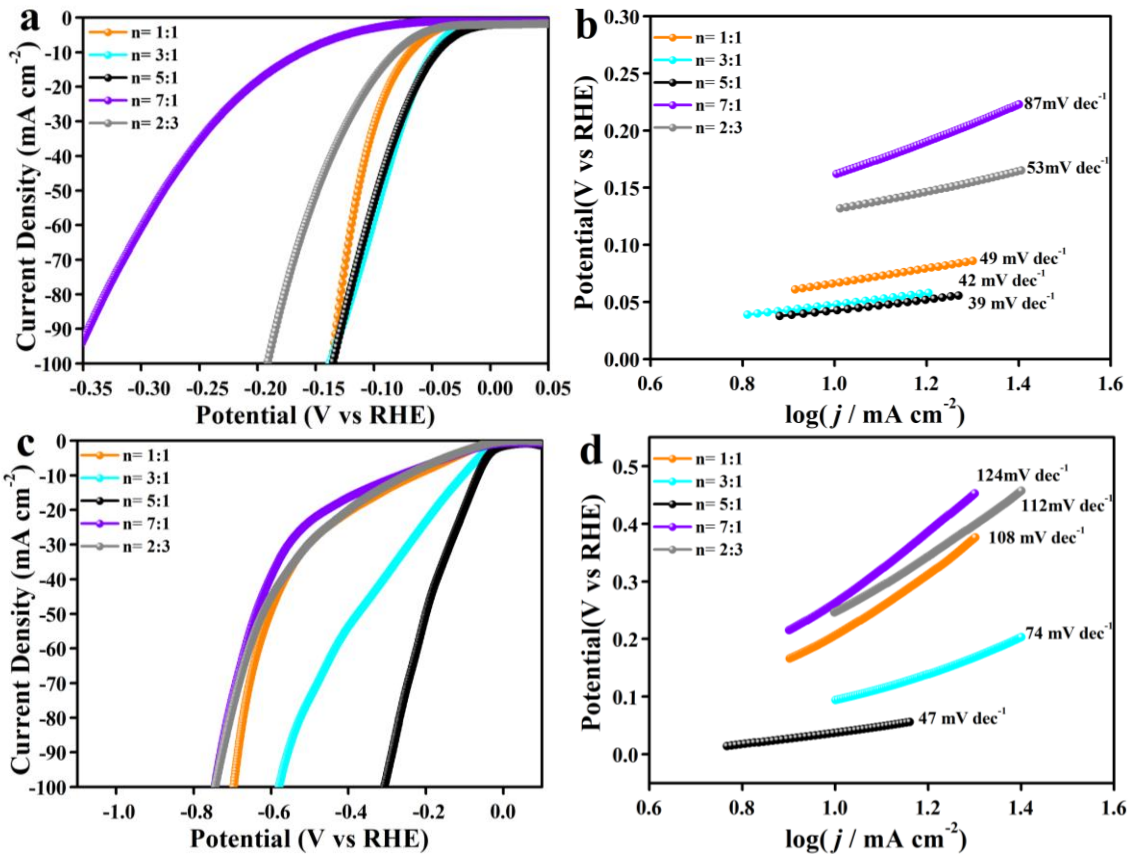

Fig. S5 The electrocatalytic performance of Ru and Cr_2O_3 with different molar ratios in Ru-Cr_2O_3/NG for HER in alkaline (1 M KOH) (a, b) and neutral medium (1 M PBS) (c, d). LSV curves (a, c); Tafel plots (b, d); n is the molar ratio of Ru to Cr_2O_3.

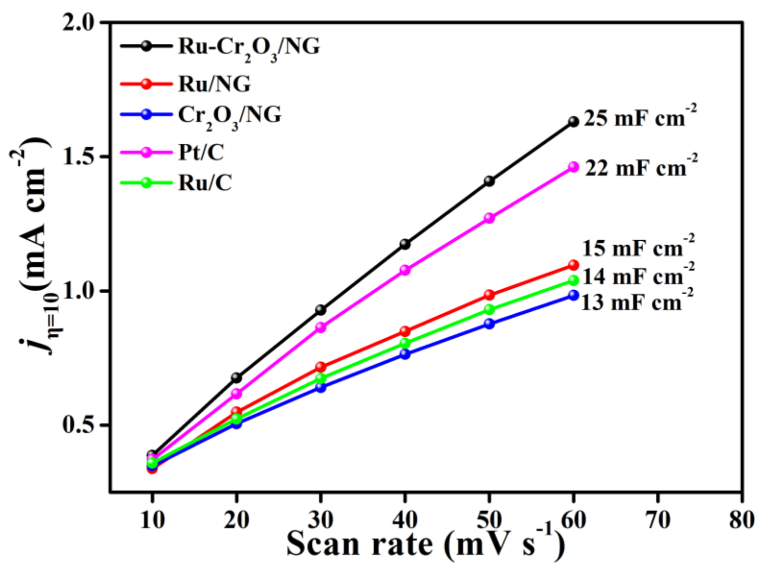

Fig. S6 The ECSA of the catalysts estimated by a double layer capacitance **(C_{dl})** measurement.

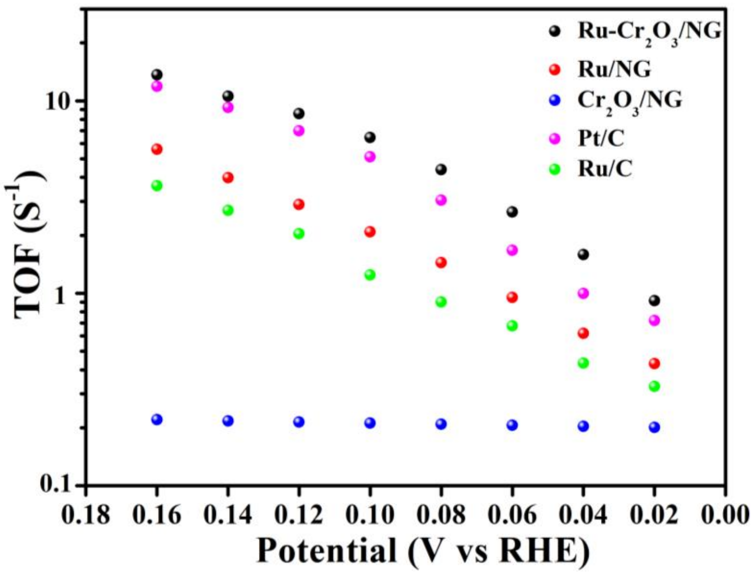

Fig. S7 TOF of Ru and Cr_2O_3 with different molar ratios in Ru-Cr_2O_3/NG, Ru/NG, Cr_2O_3/NG, 20 wt.% Pt/C and Ru/C in alkaline medium (1.0 M KOH).

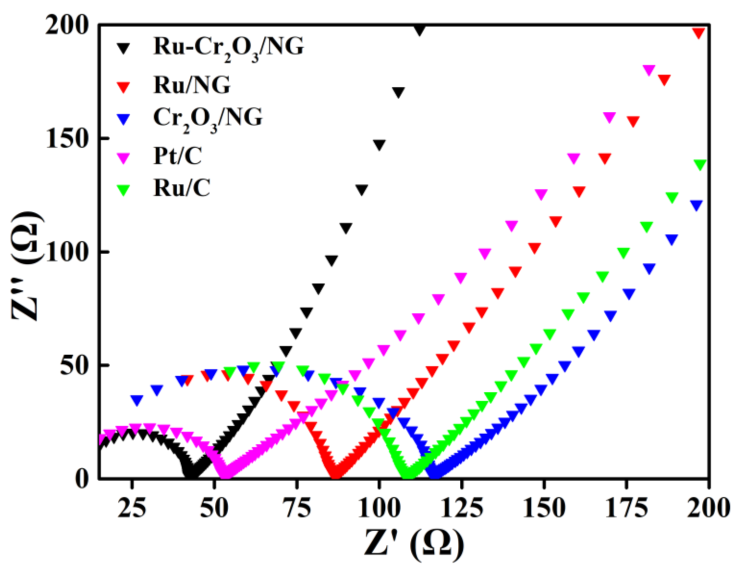

Fig. S8 The comparison of the EIS of Ru-Cr_2O_3/NG, Ru/NG, Cr_2O_3/NG, 20 wt.% Pt/C and Ru/C.

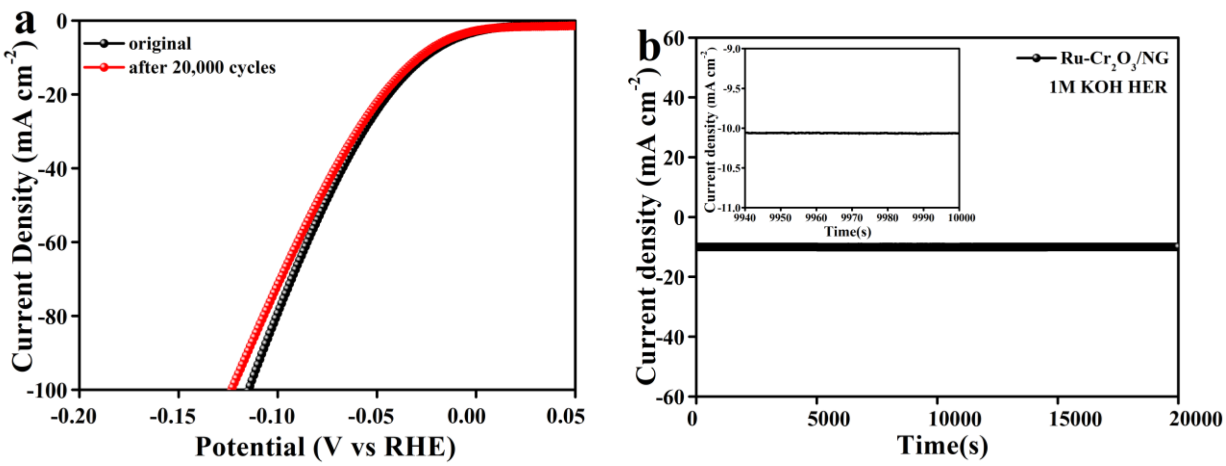

Fig. S9 The LSV curves of Ru-Cr_2O_3/NG over 20000 cycles (a) and the I-t curves of Ru-Cr_2O_3/NG (b) in alkaline medium (1.0 M KOH) at -1.073V.

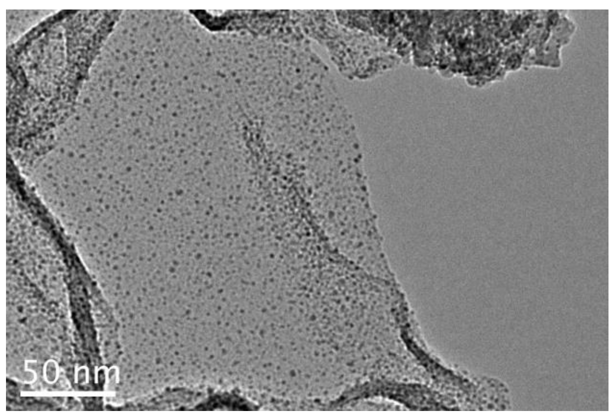

Fig. S10 TEM images of Ru-Cr_2O_3/NG after long-term test.

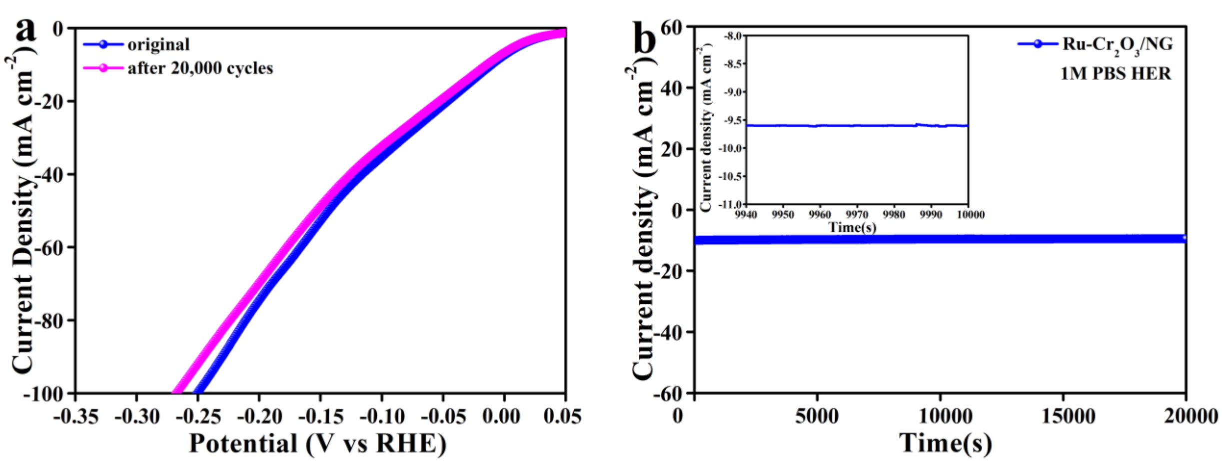

Fig. S11 The LSV curves of Ru-Cr_2O_3/NG over 20000 cycles (a) and the I-t curves of Ru-Cr_2O_3/NG (b) in neutral medium (1.0 M PBS) at -0.652V.

Tab. S1 The mass content of Ru and Cr_2O_3 on the NG

wt.% / catalyst	Ru	Cr_2O_3
Ru-Cr_2O_3/NG	17.0	1.8
Ru/NG	19.6	0
Cr_2O_3/NG	0	18.9
Ru/C	19.3	0

Tab. S2 Comparison of HER performance in alkaline/neutral media for Ru, Cr_2O_3/NG with other HER electrocatalysts.

Catalysts	**Electrolytes /(pH)**	**η10 (mV)**	**Tafel slope (mV dec^{-1})**	**TOF [a] (s^{-1})**	**Catalyst loading (mg cm^{-2})**	**Ref.**
Ru, Cr_2O_3/NG	1 M KOH	47	39	6.4	0.86	This work
	1 M PBS	53	47	-		
Ru/C_3N_4/C	0.1 M KOH	79	-	4.2	0.204	[1]
Ru/C-TiO_2	1 M KOH	44	73.7	0.0223[b]	0.2	[2]
Ru/MEOH/THF	0.1 M PBS	83	80	0.87	-	[3]
CoP@BCN	1 M KOH	122	59	-	0.4	[4]
	1 M PBS	215	52	-		
Ru/NC	1 M KOH	17	32	10.2	0.24	[5]
RuP_2@NPC	1 M KOH	52	69	-	1.0	[6]
	1 M PBS	57	87	-		
Mo_2C@2D-NPC	1 M KOH	45	46	-	0.247	[7]
MoP_2 NS/CC	1 M KOH	67	70	-	7.8	[8]
	1 M PBS	85	98.3	-		
CoP/CC	1 M KOH	209	129	-	0.92	[9]
	1 M PBS	106	93	-		
Rh_2P	1 M KOH	30	50	-	0.15	[10]
	1 M PBS	38	46	-		

[a] The values are calculated based on overpotential of 100 mV, except that b is at an overpotential of 150mV.

Tab. S3 Binding energies of H^+ and OH^- on various surfaces

Surface	ΔE_H (eV)	ΔE_{OH} (eV)
Ru	-0.15	0.20
Ru/NG	-1.18	-0.88
Ru/Cr_2O_3	-1.64	-1.26
Ru-Cr_2O_3/NG	-1.82	-2.05

References

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