

SUPPLEMENTARY INFORMATION

Dopant driven tuning of hydrogen oxidation mechanism at the pore/nickel/zirconia triple phase boundary

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Table S1: Energy barriers (eV) for the three HOR mechanisms at 1000K after different types of OCV correction.

HOR mechanism	Reaction step	Type of OCV correction	Y	Sc	Al	Ce	Ca	Y in bulk
O-migration	1-2 ^a	Any	1.26	1.27	0.87	1.36	1.26 ^b	1.80
On-boundary	4-5 ^a	Individual	1.35	1.23 ^c	1.29 ^c	1.28	1.85 ^c	1.30
		YSZ-based	1.35	1.22 ^c	1.12 ^c	1.26	1.81 ^c	1.33
		No	1.41	1.28 ^c	1.18 ^c	1.31	1.87 ^c	1.28
	7-8	Individual	0.90	1.07 ^c	0.99 ^c	1.10	1.52 ^c	1.08
		No	0.95	1.12 ^c	0.88 ^c	1.13	1.54 ^c	1.16
H-migration	4-5 ^a	Individual	1.35	1.17	1.29	1.22	1.85	1.30
	9-10 ^a	Individual	1.35	1.17	1.29	1.22	1.85	1.30

^a The step is rate-limiting for the corresponding HOR mechanism.

^b Migration of OH occurs from the nickel surface back to zirconia, which does not allow the HOR to be completed via the O-migration mechanism.

^c Dissociation of water molecule occurs at the TPB, which does not allow the HOR to be completed via the on-boundary mechanism.