Supporting Information

Improving the Carbon Resistance of Ni-based Steam Reforming Catalyst by Alloying with Rh. A Computational Study Coupled with Reforming Experiments and EXAFS Characterization

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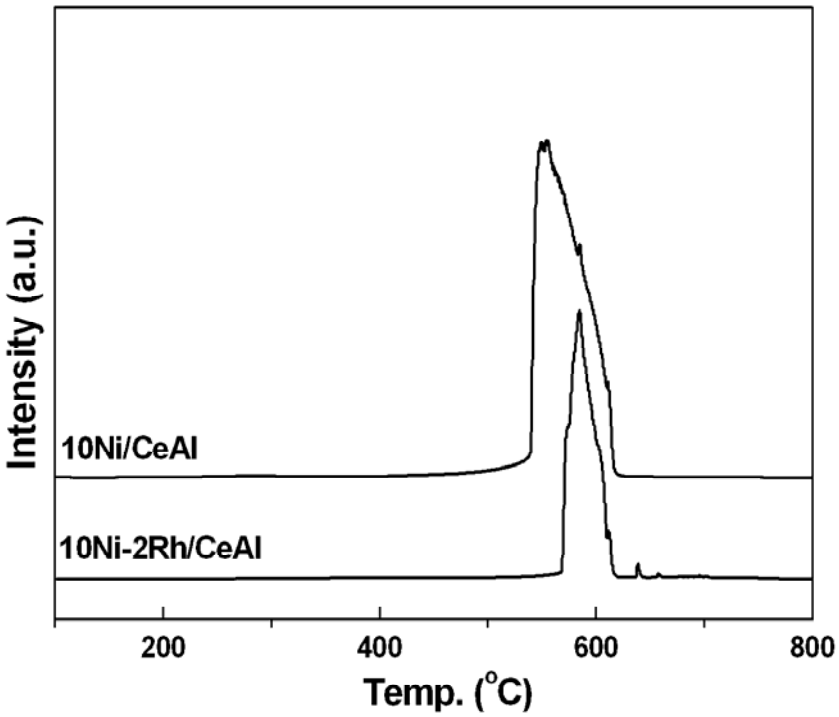

Figure S-1. TPO profiles of used 10wt%Ni/CeAl and 10wt%Ni-2wt%Rh/CeAl catalysts after steam reforming of Norpar13 at 550 °C for 55 h.

Table S-1. Calculated activation energies and reaction energies for the oxidation of hydrogenated carbon (CH-O formation) and dehydrogenated carbon (C-O formation) over (111) surfaces.

	Reaction energy (eV)	Activation energy (eV)	Relative rate *
CH-O formation			
Ni(111)	0.096	1.15	1.0
Ni_8Rh_1/Ni(111)_near	0.017	1.31	0.10
Ni_8Rh_1/Ni(111)_far	0.017	1.14	1.2
Ni_2Rh_1(111)	0.13	1.14	1.2
Rh(111)	0.12	1.37	0.045
C-O formation			
Ni(111)	-1.75	1.18	1.0
Ni_8Rh_1/Ni(111)_near	-1.83	1.41	0.039
Ni_8Rh_1/Ni(111)_far	-1.72	1.29	0.21
Ni_2Rh_1(111)	-1.66	1.16	1.3
Rh(111)	-1.43	1.37	0.069

* at a temperature of 550 °C