Supporting Information for

Synthesis of ultrathin Ni nanosheets for semihydrogenation of phenylacetylene to styrene under mild conditions

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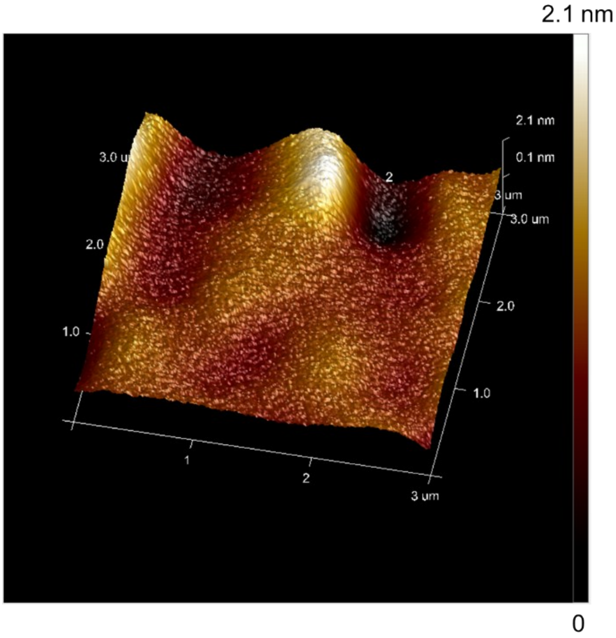

Fig. S1 AFM image of Ni NSs formed at 4 h.

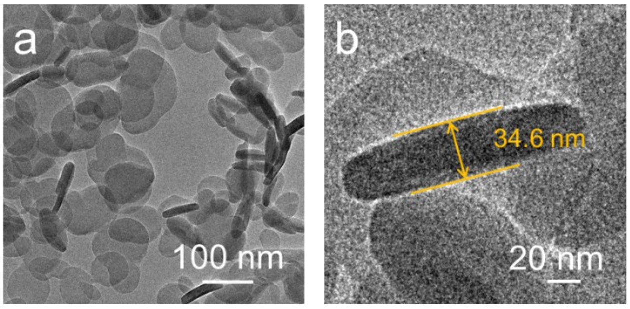

Fig. S2 TEM images of Ni NSs synthesized with no amine addition.

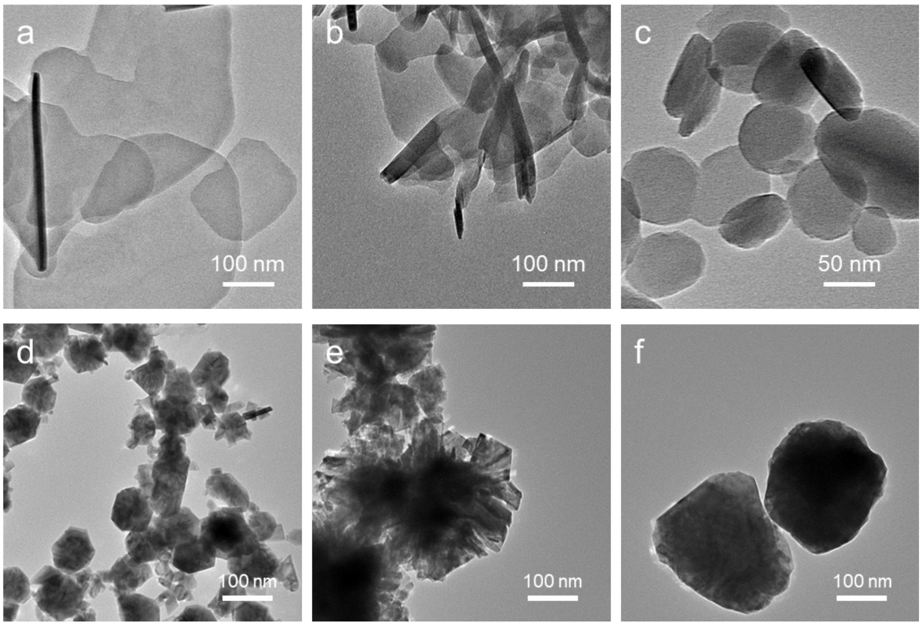

Fig. S3 TEM images of Ni NSs synthesized using (a) *n*-octylamine, (b) benzylamine, (c) triethylamine, (d) 2-butylamine, (e) cholamine and (f) ethanediamine as shape controlling reagents, respectively.

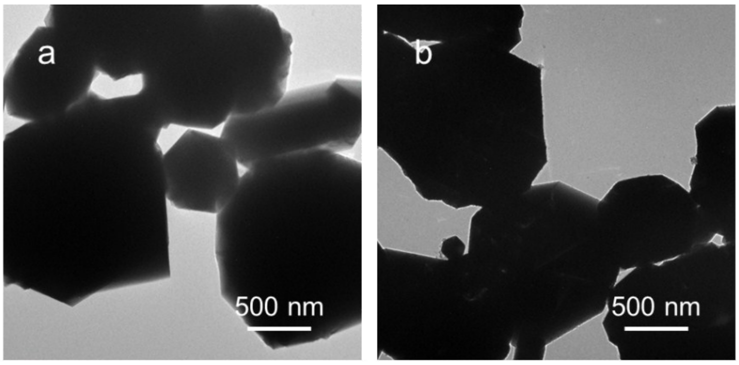

Fig. S4 TEM images of Ni NSs formed at (a) 8.5 h and (b) 18 h reaction times.

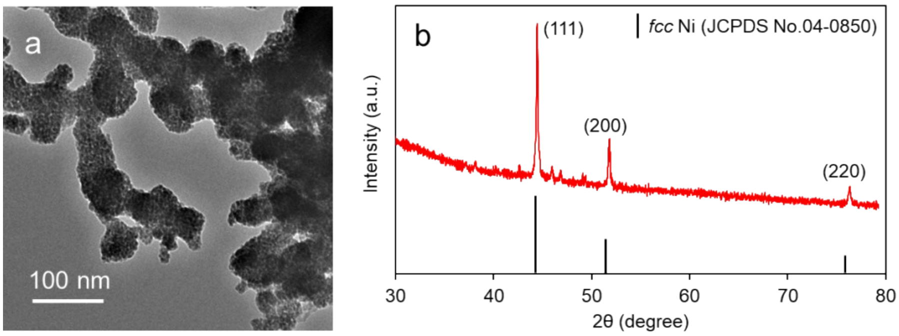

Fig. S5 (a) TEM image and (b) XRD pattern of Ni-B NPs prepared with sodium borohydride reduction method. Black vertical lines in (b) represent the standard data for *fcc* Ni (JCPDS No.04-0850).

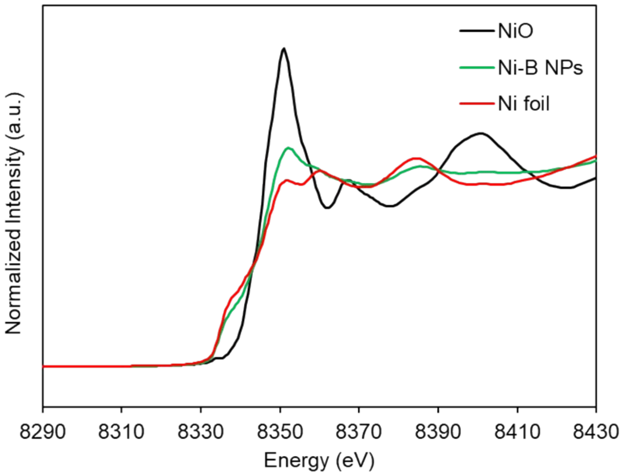

Fig. S6 XANES spectrum of Ni-B NPs compared to those of Ni foil and NiO standard samples.

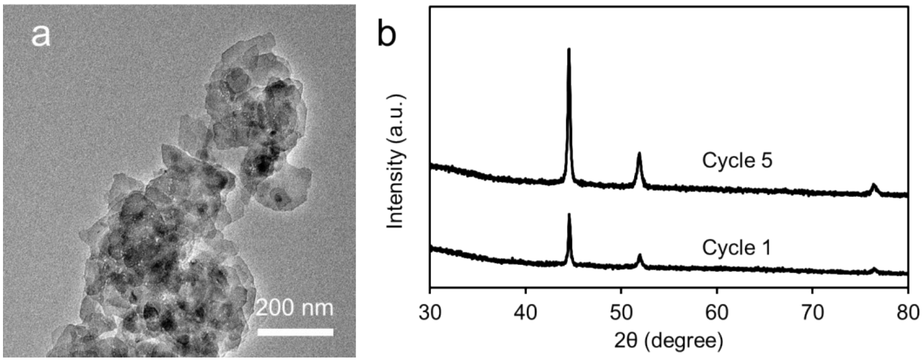

Fig. S7 (a) TEM image of Ni-4h after recycling for 5 times. (b) XRD patterns of Ni-4h after recycling for 1 and 5 times.

Table S1 EXAFS fitting results of Ni NSs formed at different solvothermal reaction times.[a]

Sample	**Coordination**	**R (Å)**	**CN**	**σ^2 (nm^2)**	**E_0 shift (eV)**	**R factor**
1h	Ni-O	2.055±0.011	4.6±0.6	0.006±0.002	-4.8	3E-3
	Ni-Ni (NiO)	3.126±0.008	5.9±0.9	0.009±0.001	-3.0	
1.5h	Ni-O	2.049±0.012	4.8±0.5	0.006±0.002	-4.1	5E-3
	Ni-Ni (NiO)	3.119±0.009	4.8±0.6	0.007±0.001	-2.3	
2h	Ni-Ni (Ni)	2.516±0.025	1.8±1.7	0.015±0.011	2.1	3E-3
	Ni-O	2.066±0.025	3.2±0.5	0.008±0.003	1.2	
	Ni-Ni (NiO)	3.130±0.010	2.0±0.6	0.004±0.002	2.1	
3h	Ni-Ni (Ni)	2.481±0.007	5.4±0.7	0.005±0.001	-6.8	2E-3
4h	Ni-Ni (Ni)	2.485±0.003	7.8±0.6	0.006±0.001	7.1	1E-3
5.5h	Ni-Ni (Ni)	2.486±0.003	9.9±0.8	0.006±0.001	3.8	1E-3

[a] R is the bond length; CN is the coordination number; σ^2 is the change in the Debye-Waller factor value relative to the reference factor; E_0 shift is inner potential correction to account for the difference in the inner potential between the sample and the reference.

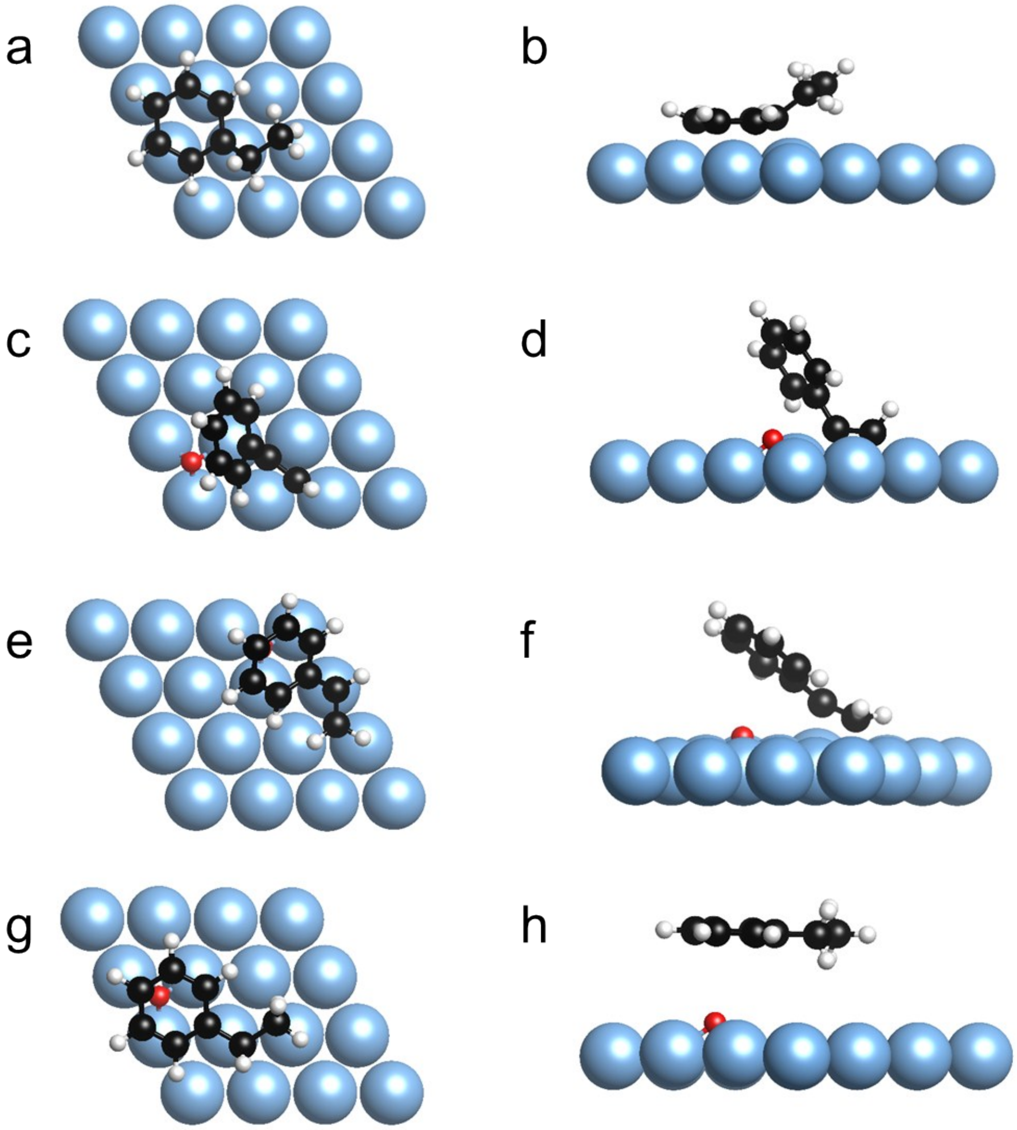

Fig. S8 Adsorption configurations of (a,b) ethylbenzene (EB) on Ni (111) and (c,d) phenylacetylene (PA), (e,f) styrene (ST), (g,h) ethylbenzene (EB) on 1/16 monolayer O covered Ni (111) surface. The blue, black, white and red balls represent modelled Ni, C, H and O atoms.

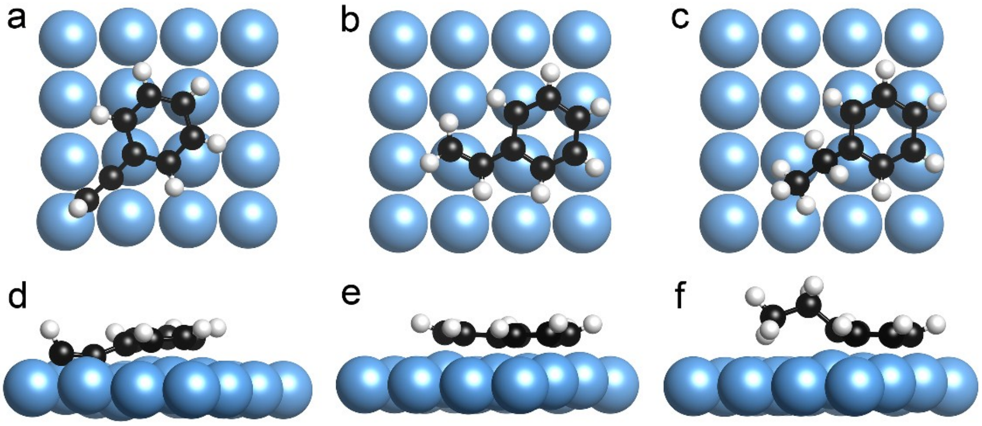

Fig. S9 Adsorption configurations of (a, d) phenylacetylene (PA), (b, e) styrene (ST), (c, f) ethylbenzene (EB) on Ni (100) surface. The blue, black, white balls represent modelled Ni, C and H atoms.

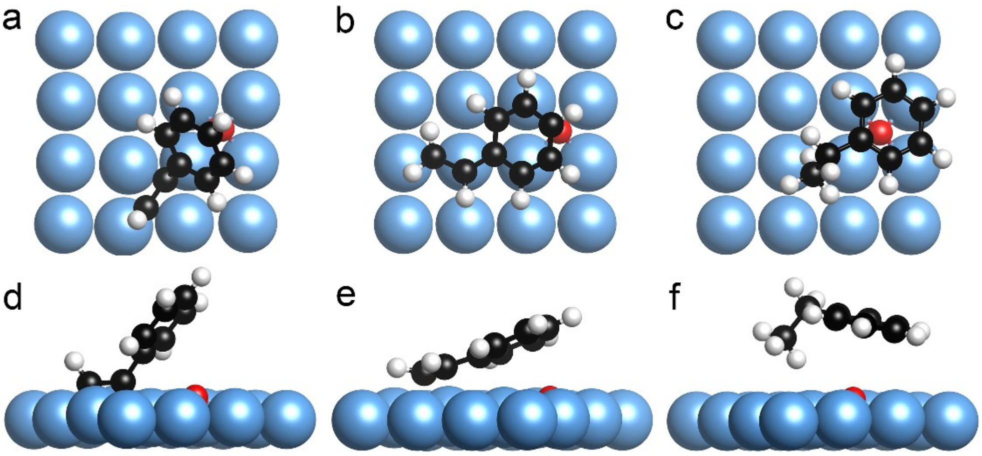

Fig. S10 Adsorption configurations of (a, d) phenylacetylene (PA), (b, e) styrene (ST), (c, f) ethylbenzene (EB) on 1/16 monolayer O covered Ni (100) surface. The blue, black, white and red balls represent modelled Ni, C, H and O atoms.

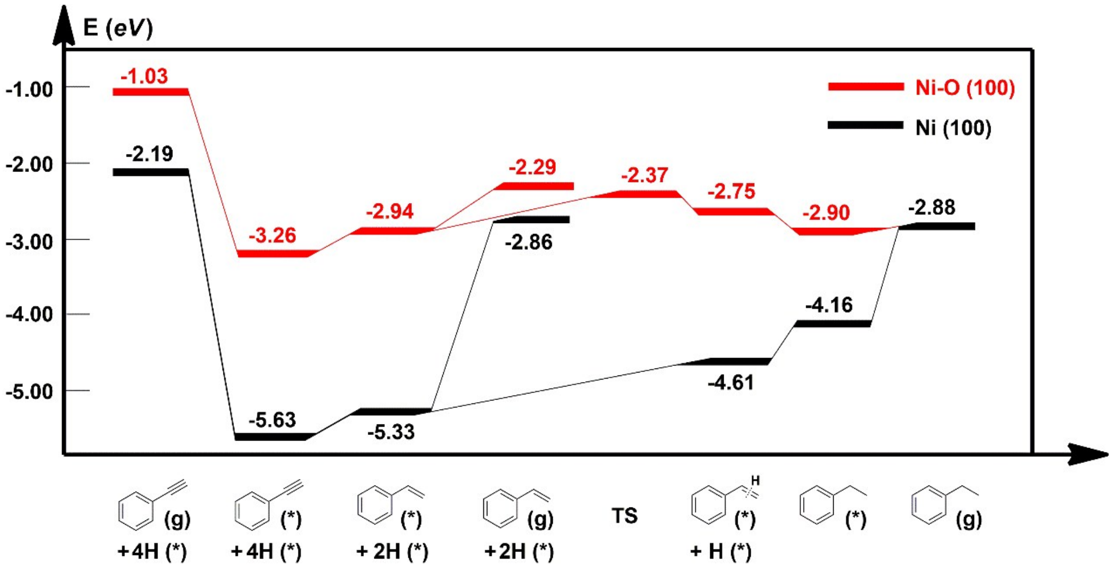

Fig. S11 Schematic potential surface of PA semihydrogenation on Ni(100) and Ni(100) with 1/16 ML oxygen coverage. (*) represents the adsorbed intermediates, and (g) represents the gas phase intermediates and products. All zero-point correlated energies are with respect to the gas phase PA and two gas phase hydrogen molecules (0 eV). TS represents the transition state.