

Supplementary Information for

A facile approach to enhancing activity of Ni₂P/SiO₂ catalyst for hydrodechlorination of chlorobenzene: promoting effect of water or oxygen

Jixiang Chen*, Ti Guo, Kelun Li, Lingmin Sun

Table 1S Properties of Ni₂P/SiO₂ before and after pretreatment

Catalyst	S _{BET} (m ² /g)	Pore volume (cm ³ /g)	Mean pore diameter(nm)	Ni content (wt.%)	Ni/P molar ratio	Ni ₂ P particle size(nm) ^a
Ni ₂ P/SiO ₂	294	0.43	5.9	12.7	1.5	12.6
Ni ₂ P/SiO ₂ -513	292	0.42	5.7	13.7	1.6	13.5
Ni ₂ P/SiO ₂ -543	297	0.43	5.8	13.7	1.6	13.8
Ni ₂ P/SiO ₂ -573	288	0.41	5.7	13.7	1.5	14.0
Ni ₂ P/SiO ₂ -673	290	0.42	5.7	13.7	1.5	15.5

^a Calculated by Scherrer equation on the base of Ni₂P(111) reflection ($2\theta=40.8^\circ$).

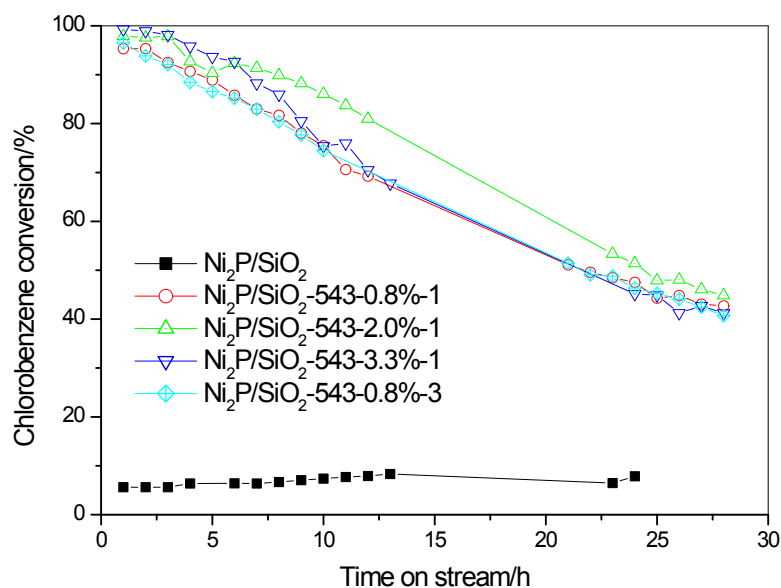


Fig. 1S Activity of Ni₂P/SiO₂ treated with a H₂O/H₂ flow.

The treated catalysts are denoted as Ni₂P/SiO₂-T-c%-t, where T, c% and t represent treatment temperature (K), water concentration in H₂ and treatment time (h).

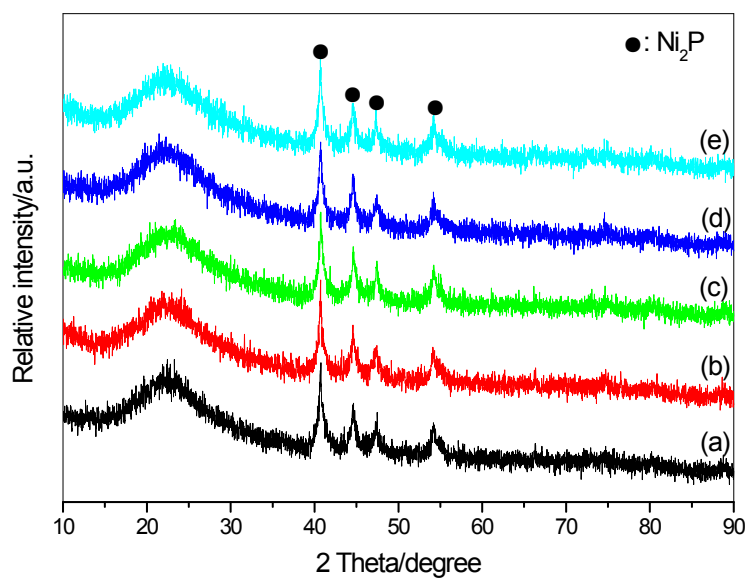


Fig. 2S XRD patterns of (a) $\text{Ni}_2\text{P}/\text{SiO}_2$; (b) $\text{Ni}_2\text{P}/\text{SiO}_2$ -513; (c) $\text{Ni}_2\text{P}/\text{SiO}_2$ -543; (d) $\text{Ni}_2\text{P}/\text{SiO}_2$ -573; (e) $\text{Ni}_2\text{P}/\text{SiO}_2$ -673

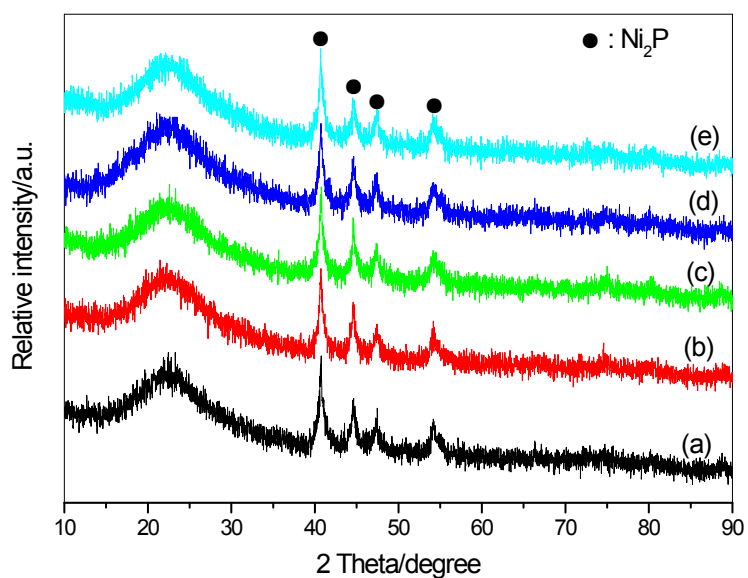


Fig. 3S XRD patterns of (a) $\text{Ni}_2\text{P}/\text{SiO}_2$; (b) $\text{Ni}_2\text{P}/\text{SiO}_2$ -270-0.8%-1; (c) $\text{Ni}_2\text{P}/\text{SiO}_2$ -270-2.0%-1; (d) $\text{Ni}_2\text{P}/\text{SiO}_2$ -270-3.3%-1; (e) $\text{Ni}_2\text{P}/\text{SiO}_2$ -270-0.8%-3

The treated catalysts are denoted as $\text{Ni}_2\text{P}/\text{SiO}_2$ -T-c%-t, where T, c% and t represent treatment temperature (K), water concentration in H_2 and treatment time (h).

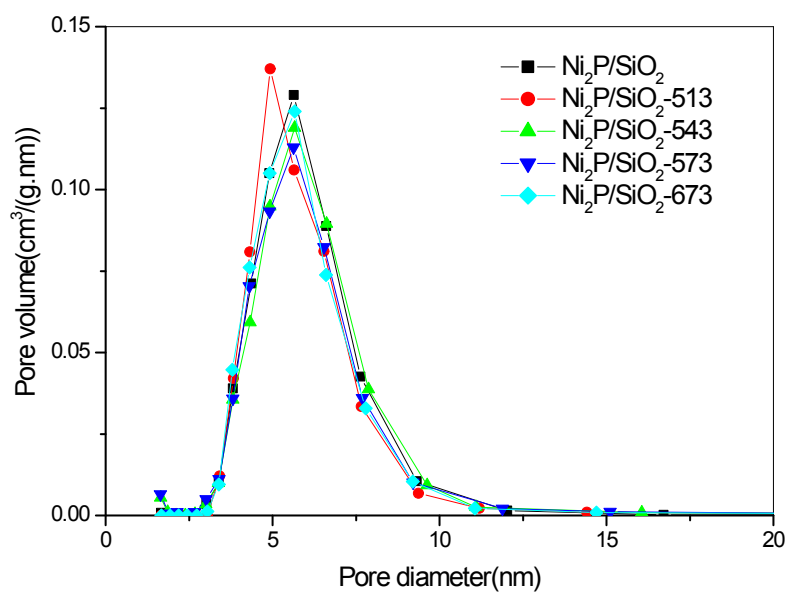
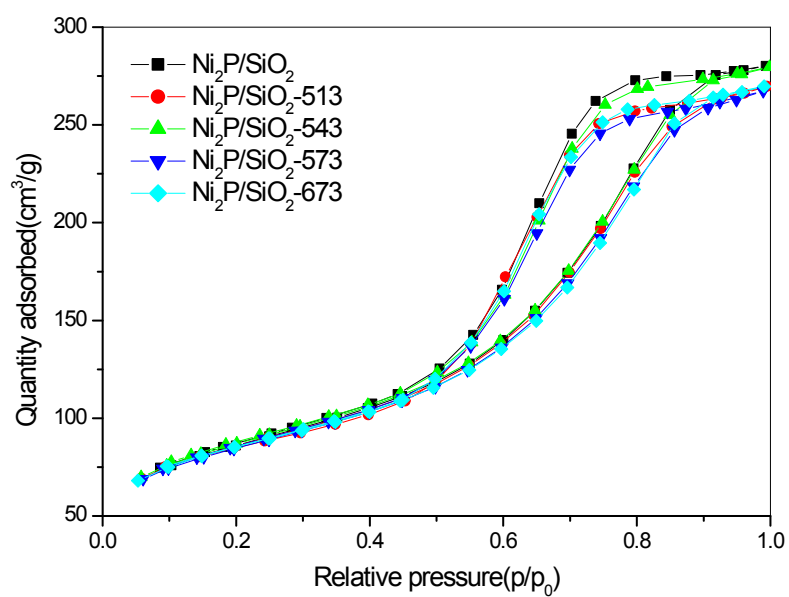
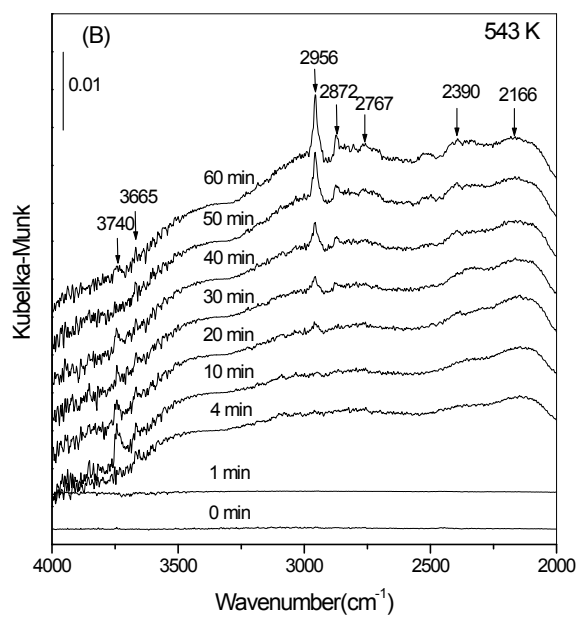
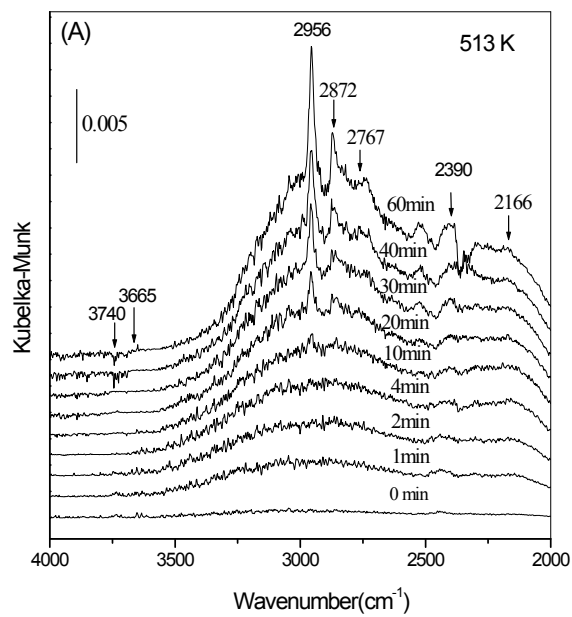


Fig. 4S Adsorption-desorption isotherms (A) and pore diameter distributions (B) of $\text{Ni}_2\text{P}/\text{SiO}_2$ and $\text{Ni}_2\text{P}/\text{SiO}_2\text{-T}$.



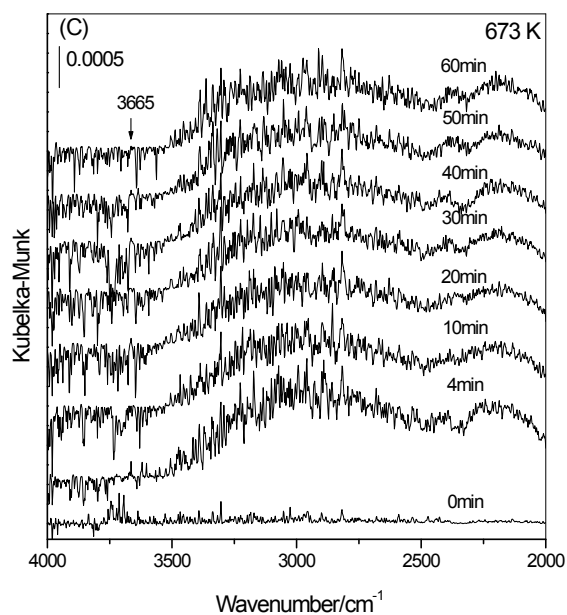


Fig. 5S In situ DRIFTS spectra of re-reduced Ni₂P/SiO₂(O₂) treated with 0.8% H₂O/H₂ at (A) 513 K; (B) 543 K and (C) 673 K

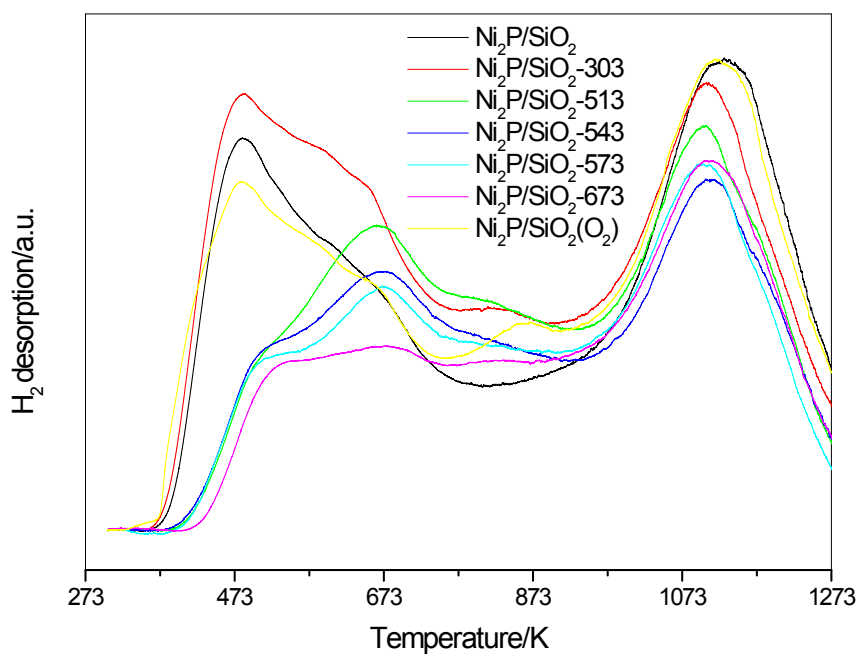


Fig. 6S H₂-TPD profiles of Ni₂P/SiO₂, Ni₂P/SiO₂-T and re-reduced Ni₂P/SiO₂(O₂)

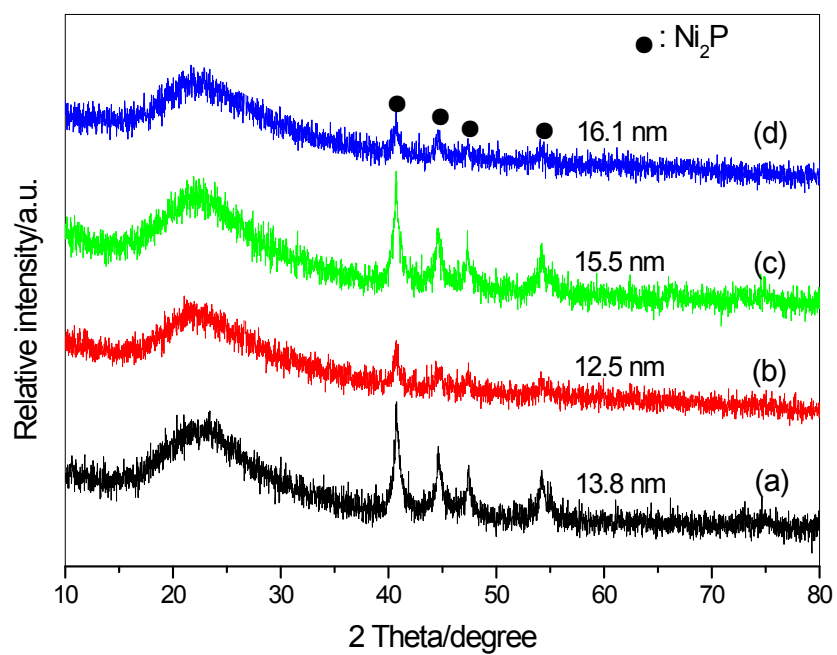


Fig. 7S XRD patterns of (a) Ni₂P/SiO₂; (b) used Ni₂P/SiO₂-543; (c) Ni₂P/SiO₂-673 and (d) used Ni₂P/SiO₂-673

Note: the figure on each pattern is the Ni₂P crystallite size calculated by Scherrer equation on the base of Ni₂P(111) reflection ($2\theta=40.8^\circ$).