Supporting Information

Solvent-Free Recycling of Polystyrene Waste into Valuable Mono-aromatics over Ni/NbO_x Catalyst

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Supporting information content

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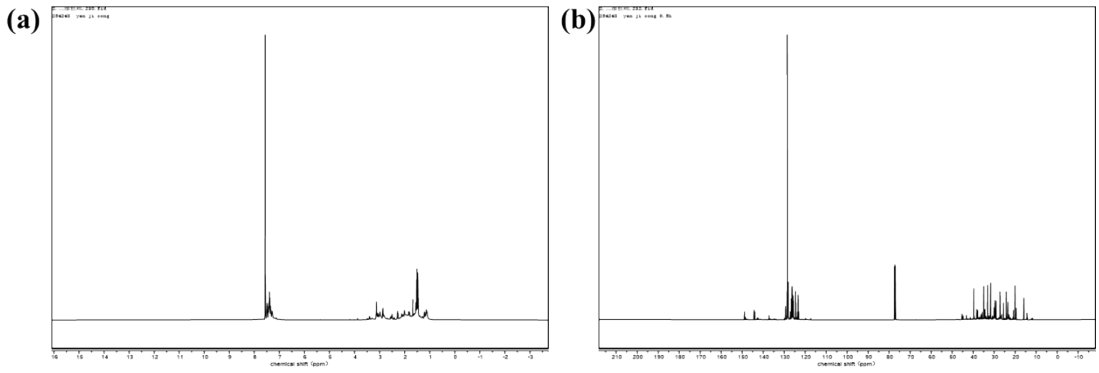


Figure S1 NMR spectra of liquid product of 1Ni/NbO_x. (a, and b, 1H and 13C NMR regions, respectively.)

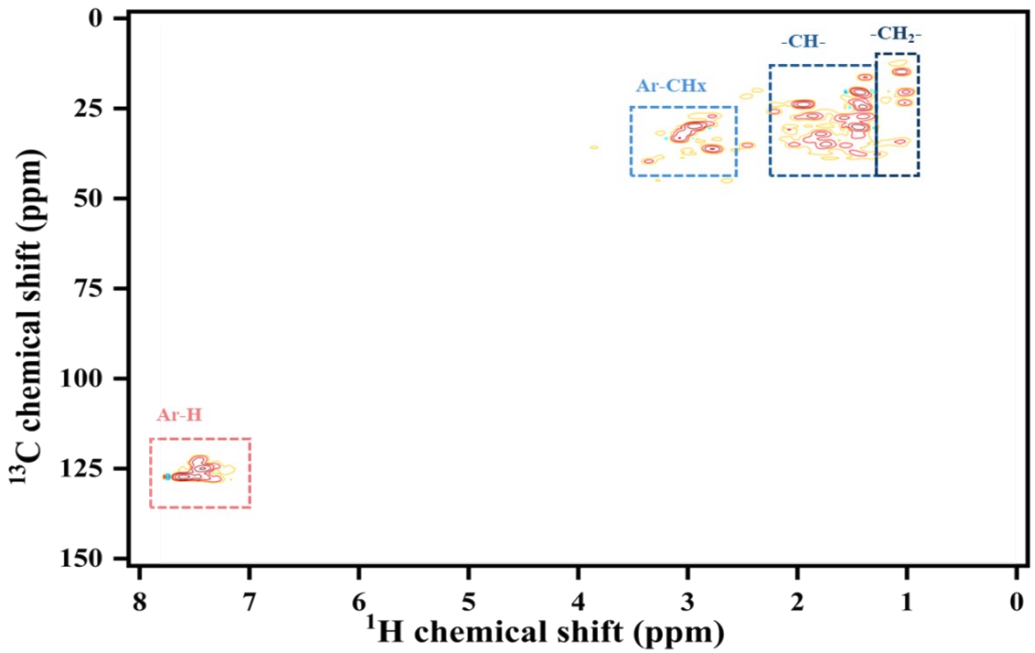


Figure S2 $^{13}C-^{1}H$ HSQC NMR of liquid product of 1Ni/NbO_x

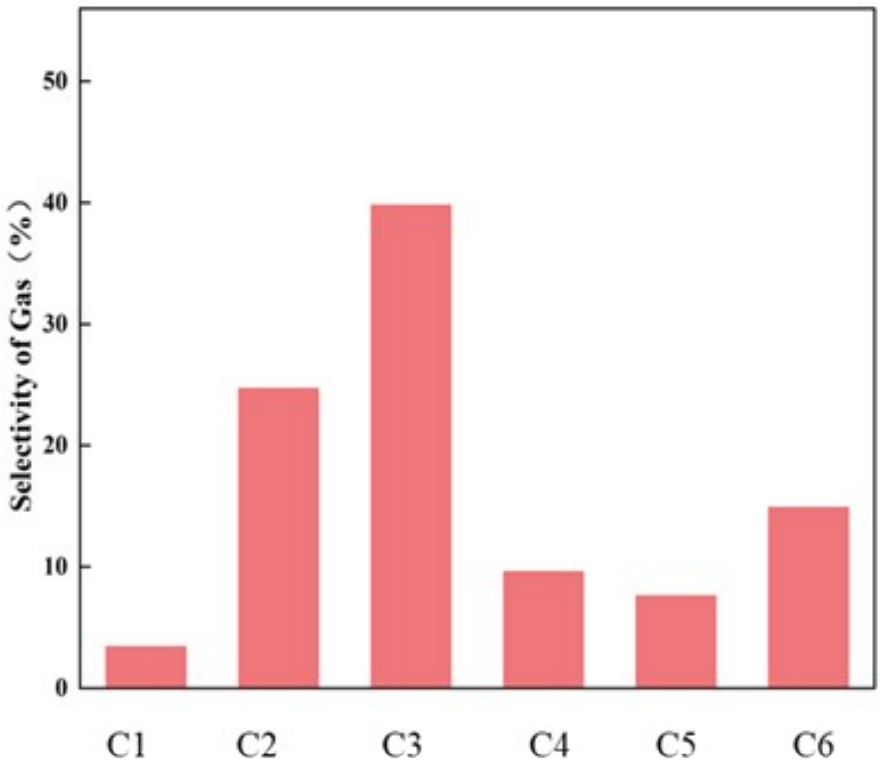
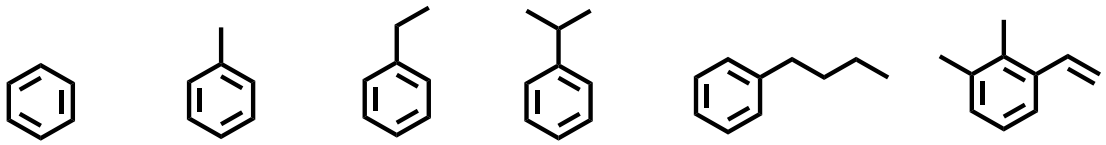
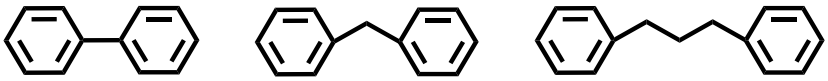


Figure S3 Gas product of 1Ni/NbO_x, reaction conditions: 260 °C, 3、24 h, and 3 MPa H_2, 4g PS, 0.4g catalyst.
Note：The gas yield is 7.57%

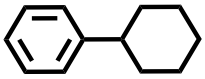
1. **Mono-aromatics**



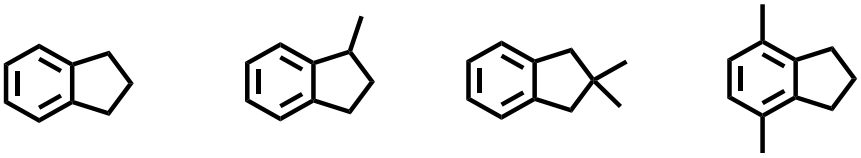
2. **Diphenyl alkanes**



3. **Hydrogenated derivatives of multiphenyl alkanes**



4. **Alkyl-substituted indanes**



5. **Alkyl-substituted tetralins**

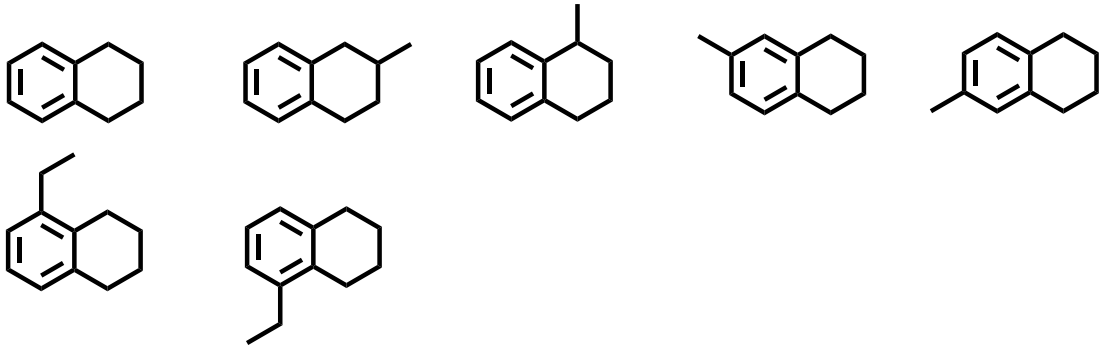


Figure S4 Structural formulas of different products

Entry	Catalyst	Temp. / °C	P. of H_2/ MPa	Time / h	Solvent	R ($g_{alkylbenzenes}$ / $g_{cat.}$ / h)	Ref.
1	Ni/NbO_x	260	3	3	-	2.02	This work
2	MoS_x-Hbeta	250	3	20	-	1.445	[1]
3	Ru/SiO_2	280	-	6	CH_3OH	1.405	[2]
4	$NbOPO_4$	280	0.5	12	Octane	0.081	[3]
5	Ru/NbO_x	300	0.5	16	Octane	0.0124	[4]
6	Ru/TiO_2	300	-	20	Decane	0.04	[5]
7	Ni/SiO_2	300	7	6	-	1.3	[6]

Table S1 Comparison of the formation rate of mono-aromatics of various catalysts for hydrocracking and hydrogenolysis of PS.

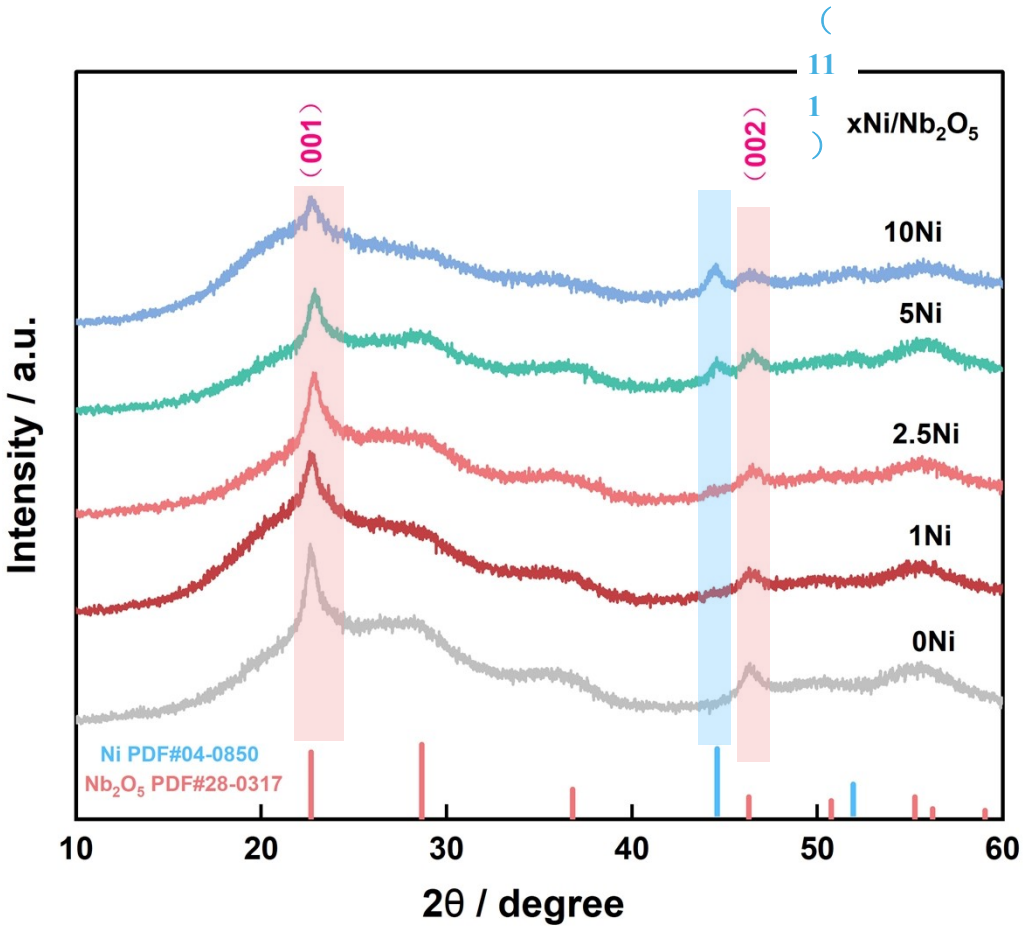


Figure S5 XRD patterns of Ni/NbO_x and standard cards.

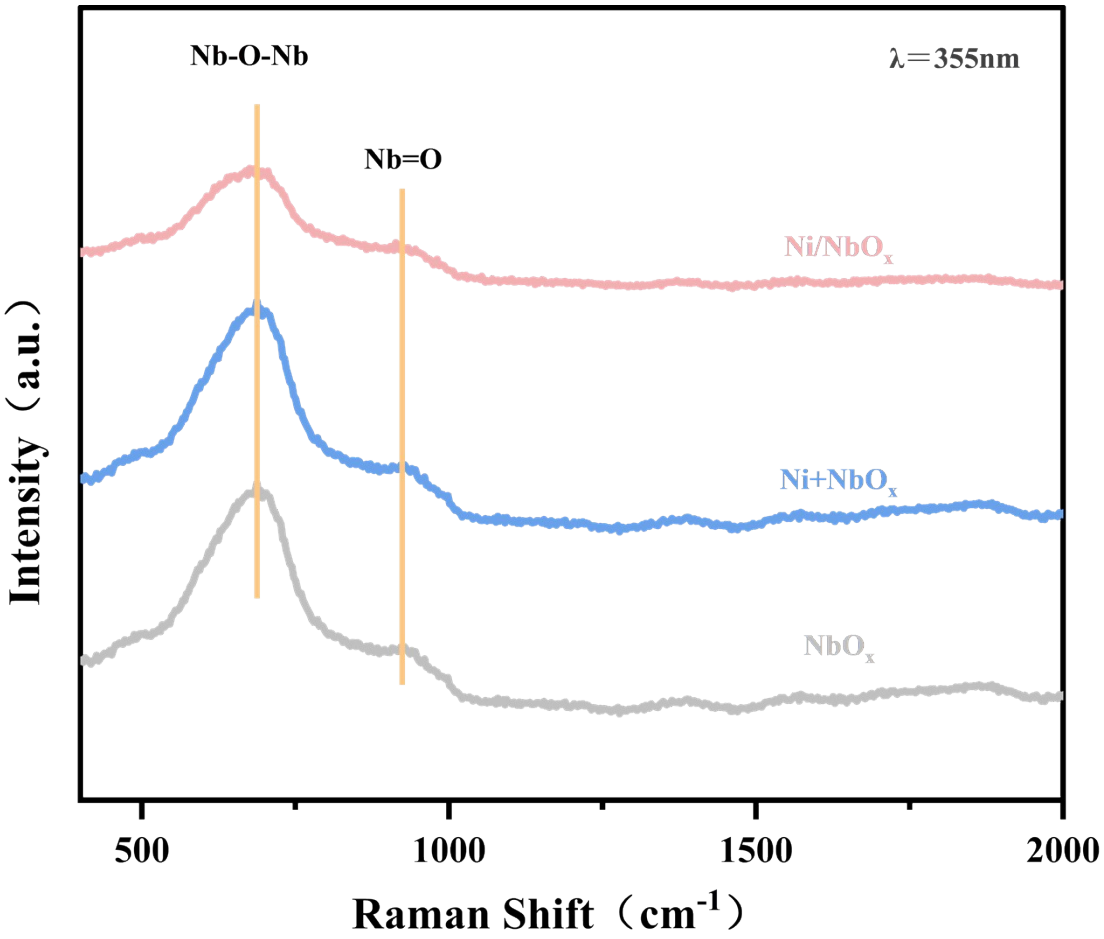


Figure S6. Raman spectroscopy of Ni/NbO_x.

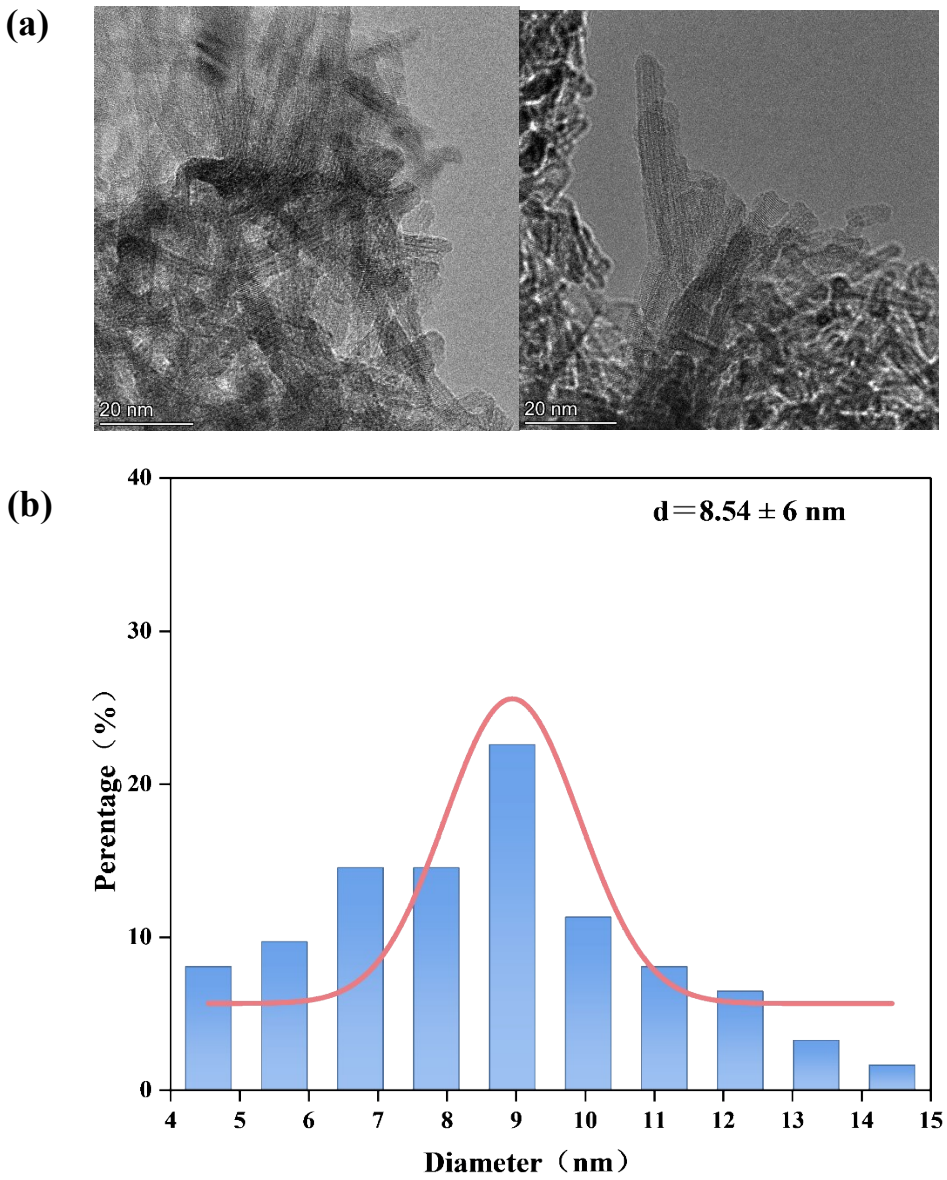


Figure S7 （a）TEM imagesand（b）their corresponding particle size distributions of 1Ni/NbO_x.

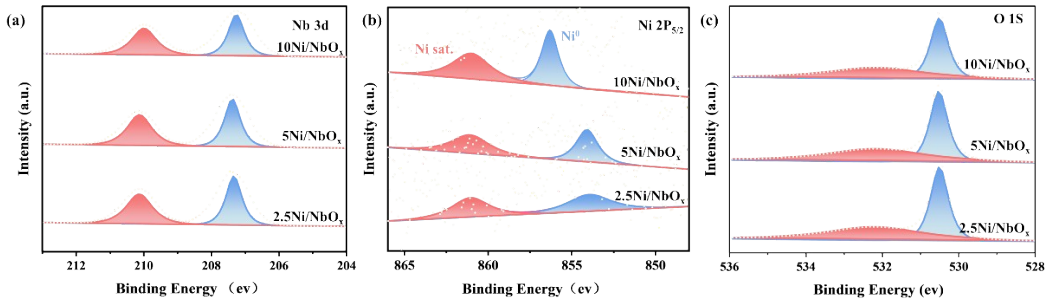


Figure S8 (a-c) Nb 3d, Ni $2P_{1/2}$, O 1S XPS spectra of 2.5、5、10 Ni/NbO_x;

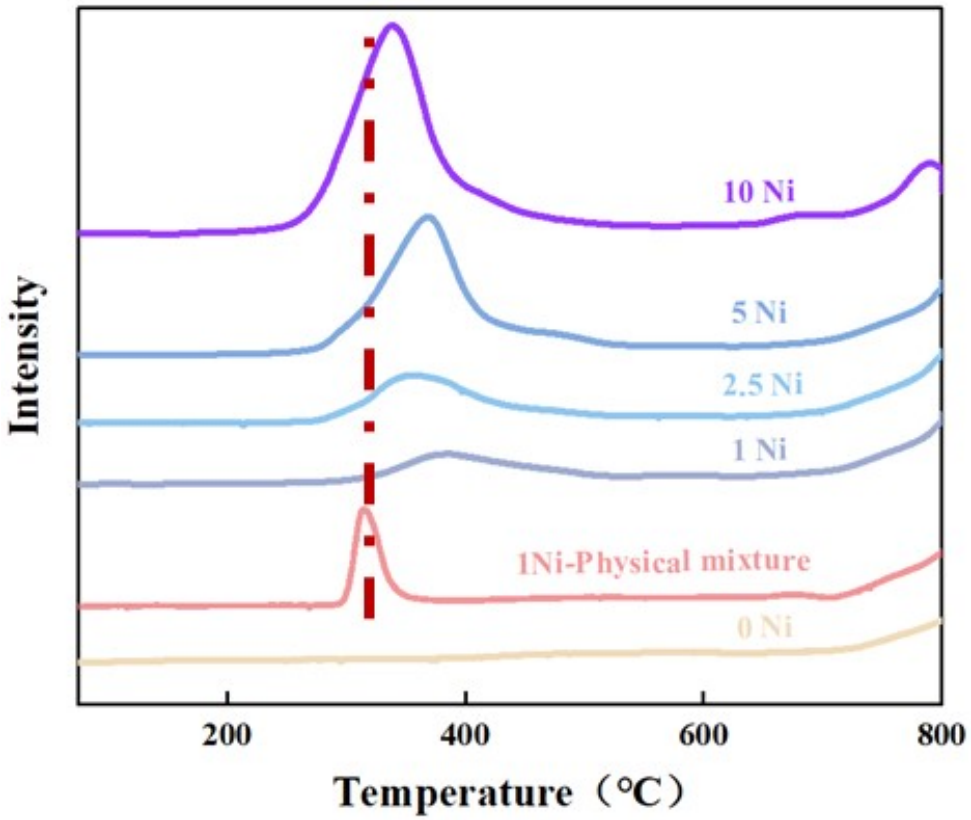


Figure S9 H_2-TPR profiles of 1-10Ni+NbO_x ,1Ni/NbO_x and NbO_x;

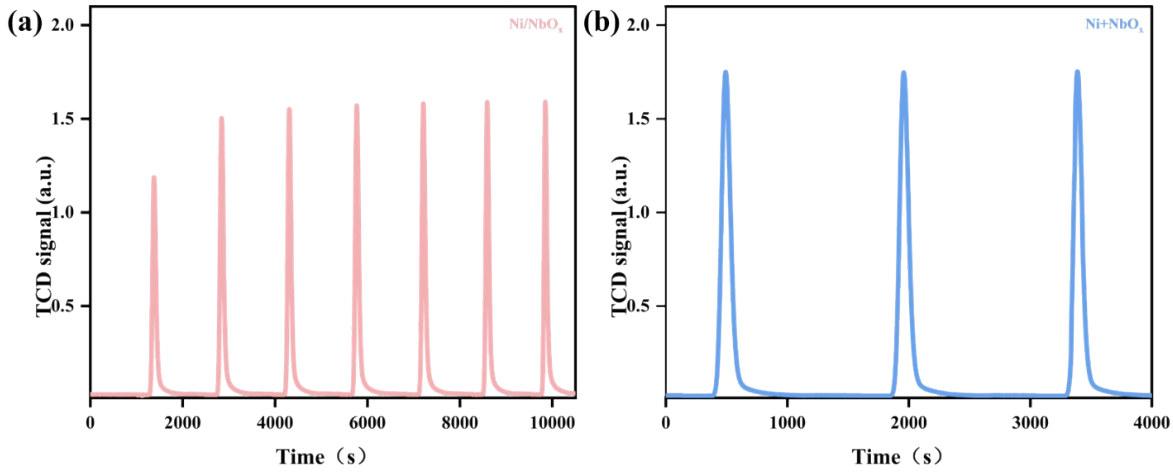


Figure S10 (a-b) H_2 Pulse Experiment of 1Ni+NbO_x and 1Ni/NbO_x.

Note：

The number of surface-exposed Ni atoms was calculated assuming dissociative adsorption of hydrogen on metallic Ni with a stoichiometry of $H/Ni_{surf} = 1$, corresponding to one hydrogen atom adsorbed per surface Ni atom. Accordingly, one molecule of H_2 was assumed to account for two surface Ni atoms. The surface Ni amount (μmol g^{-1}) was therefore calculated as twice the measured H_2 uptake.

The total amount of Ni atoms was determined from the nominal Ni loading and the molar mass of Ni (58.69 g mol^{-1}). Ni dispersion (D) was calculated as the ratio of surface Ni atoms to total Ni atoms according to the following equation:

$$D\ (\%) = \frac{2 \times nH_2}{(W_{Ni}/100)/58.69} \times 100\%$$

where n_{H_2} is the measured H_2 uptake (μmol g^{-1}) and w_{Ni} is the Ni loading (wt%).

It should be noted that for Ni supported on NbOx, strong metal–support interactions and incomplete reduction may suppress hydrogen adsorption, leading to an underestimation of the absolute Ni dispersion.

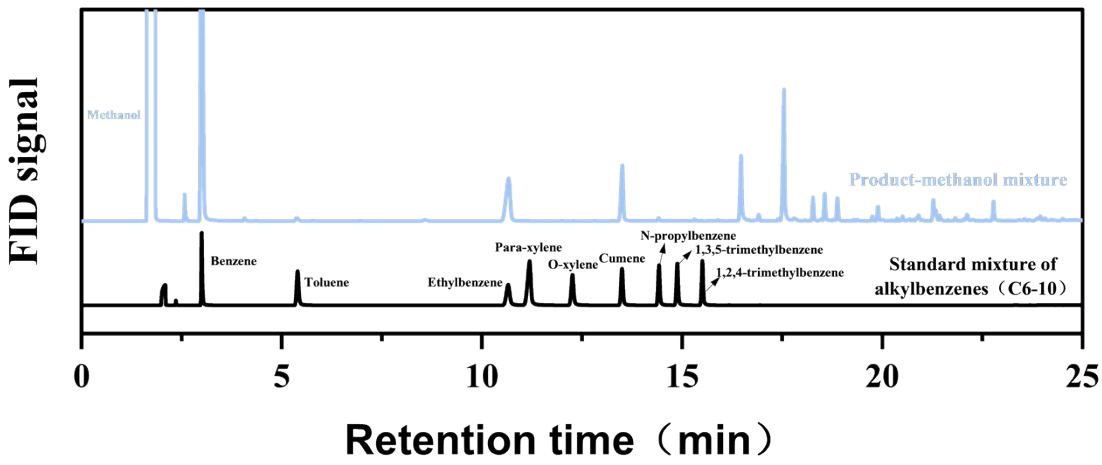


Figure S11. GC chromatogram recorded using an FID detector of gas products from the reaction of PS over 1Ni/NbO_x at 260 ℃ under 3 MPa of H_2 for 3 hours

References:

[1] Zhang, G.; Mao, Q.; Yue, Y.; Gao, R.; Duan, Y.; Du, H. Ni-based catalysts supported on Hbeta zeolite for the hydrocracking of waste polyolefins. *RSC Advances* **2024**, *14* (23), 15856-15861. DOI: 10.1039/d4ra02809k.

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[3] Zhou, H.; Chen, L.; Guo, Y.; Liu, X.; Wu, X.-P.; Gong, X.-Q.; Wang, Y. Hydrogenolysis Cleavage of the C_{sp2}–C_{sp3} Bond over a Metal-Free NbOPO4 Catalyst. *ACS Catalysis* **2022**, *12* (9), 4806-4812. DOI: 10.1021/acscatal.2c00034.

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