Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Identification of electron-rich mononuclear Ni atoms on TiO_2-A distinguished from Ni particles on TiO_2-R in guaiacol hydrodeoxygenation pathways

Xiaoqiang Zhang [a,b], Peifang Yan [a], Bin Zhao [c], Z. Conrad Zhang*[a]

[a]State Key Laboratory of Catalysis, Dalian National Laboratory for Clean Energy, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, P. R. China

[b]University of Chinese Academy of Sciences, Beijing 10049, P. R. China

[c]State Key Laboratory of Fine Chemicals, PSU-DUT Joint Center for Energy Research, School of Chemical Engineering, Dalian University of Technology, Dalian 116024, P. R. China

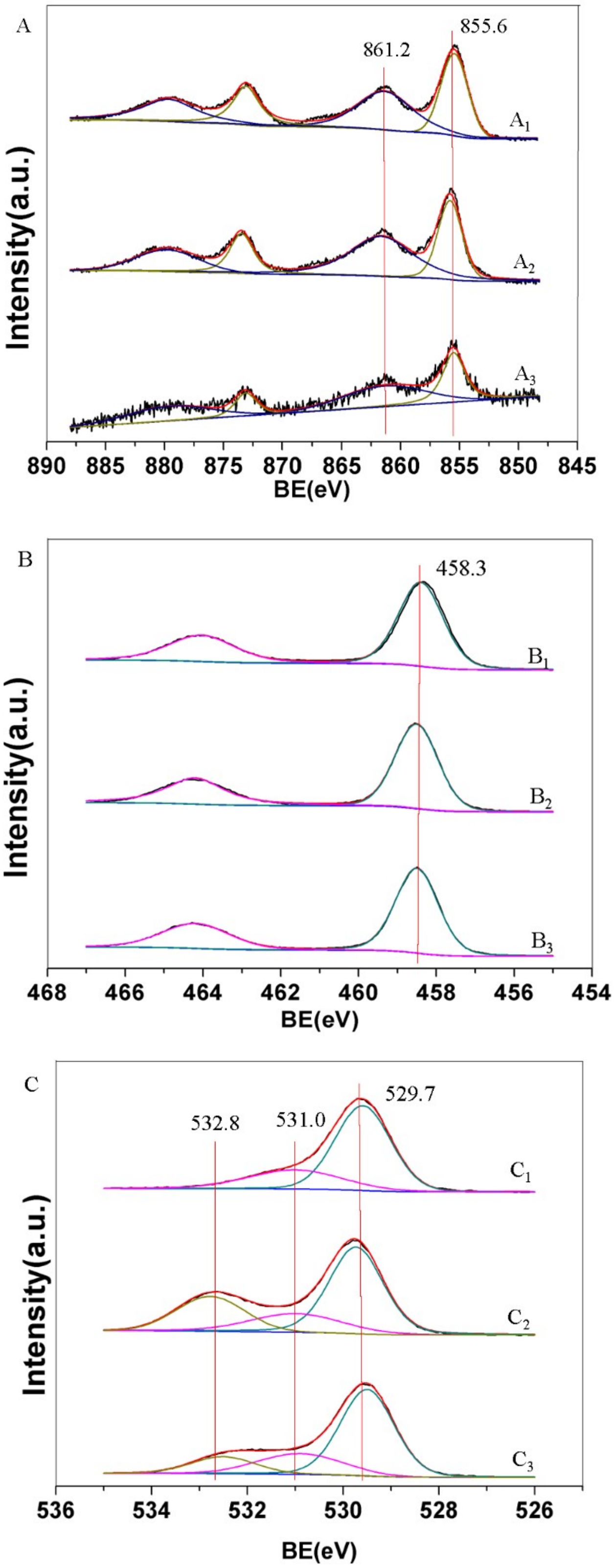

Figure S1. (A) XPS spectra Ni 2p of (A_1) 3%Ni/TiO_2-R, (A_2) 3%Ni/TiO_2-A, (A_3) 0.5%Ni/TiO_2-A; (B) XPS spectra Ti 2p of (B_1) 3%Ni/TiO_2-R, (B_2) 3%Ni/TiO_2-A, (B_3) 0.5%Ni/TiO_2-A; (C) XPS spectra O 1s of (C_1) 3%Ni/TiO_2-R, (C_2) 3%Ni/TiO_2-A, (C_3) 0.5%Ni/TiO_2-A.

Table S1. Ni loading of the supported Ni catalysts

Sample	Ni (wt. %)[a]
0.1%Ni/TiO_2-A	0.09
0.2%Ni/TiO_2-A	0.18
0.3%Ni/TiO_2-A	0.28
0.4%Ni/TiO_2-A	0.36
0.5%Ni/TiO_2-A	0.47

[a] Measured by ICP-OES

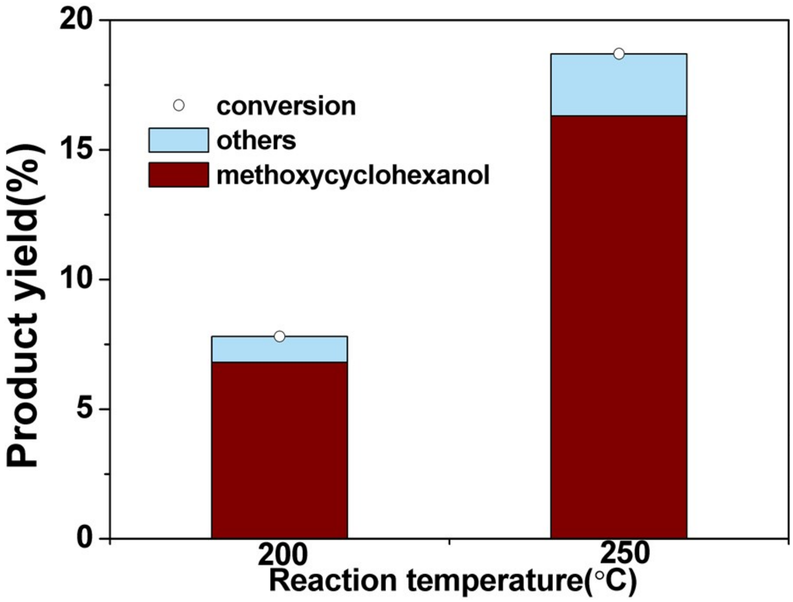

Figure S2. Product yields in guaiacol hydrogenation over 0.5%Ni/TiO_2-R 400/1h catalysts. “Others” corresponding to unidentified C_{8+} heavier products are calculated based on mass balance. Reaction condition: guaiacol 1.20 g, decane 25 mL, P (H_2) = 4 MPa, 500 rpm, 2 h. Guaiacol conversion is plotted on the same scale.

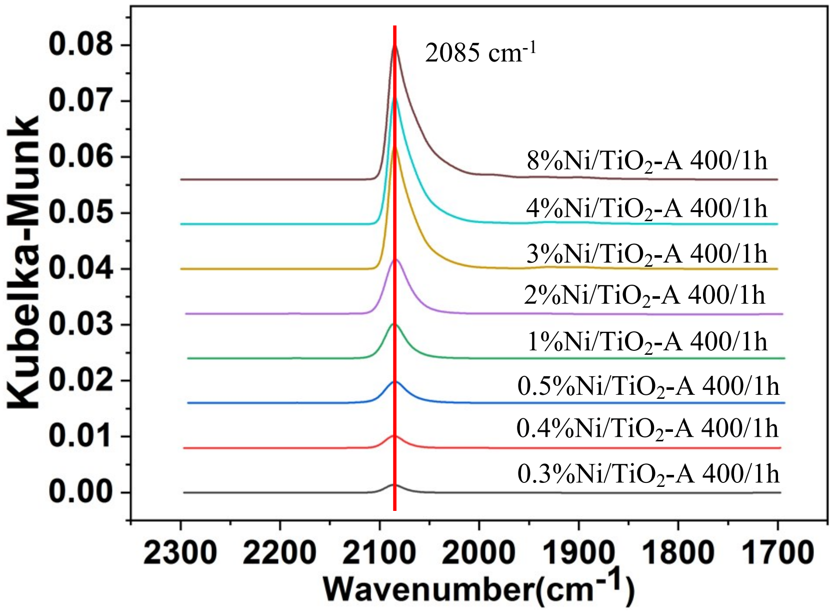

Figure S3. *In-situ* DRIFT spectra of Ni/TiO_2-A 400/1h with different Ni loadings upon CO chemisorption at 30 °C

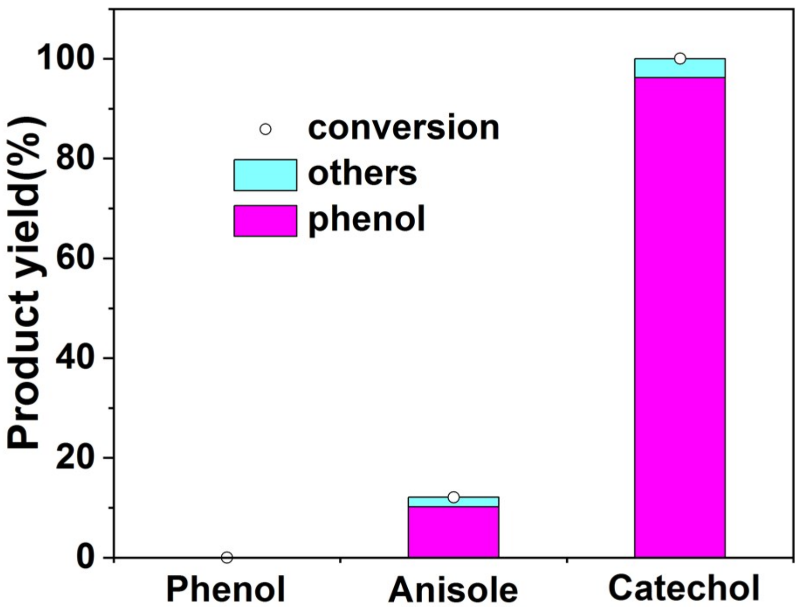

Figure S4. Product yields in other lignin-derived bio-oils (phenol, anisole and catechol) hydrogenation over 3%Ni/TiO_2-A 400/1h. “Others” corresponding to unidentified heavier products are calculated based on mass balance. Reaction condition: reactant 1.20 g, decane 25 mL, P (H_2) = 4 MPa, 500 rpm, 2 h.