Supporting information

The role of Ni sites located in mesopores for the selectivity of anisole hydrodeoxygenation

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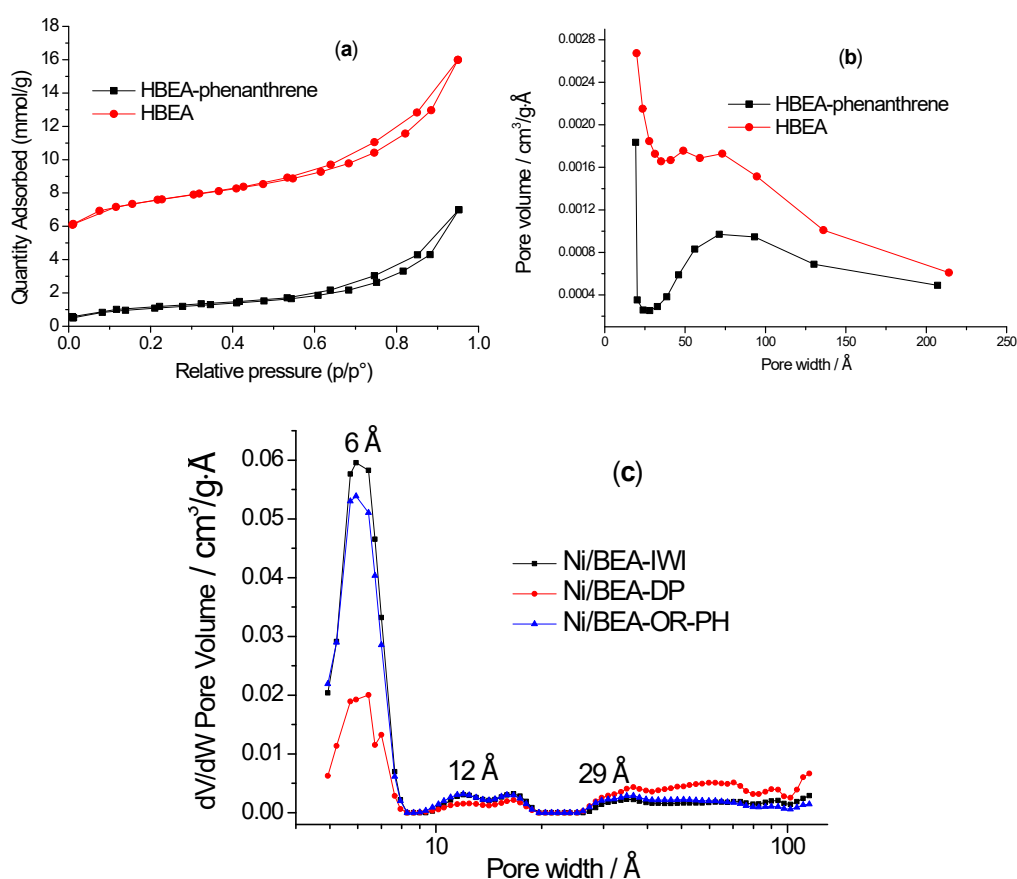**Corresponding author:** michael.stockenhuber@newcastle.edu.au

Figure S1. (**a**) N_2 adsorption-desorption isotherms and (**b**) pore size distribution of HBEA and HBEA following phenanthrene exposure; (**c**) Ar-NLDFT pore size distribution of Ni/BEA catalysts from the argon (-196 °C) isotherms.

Table S1. Acid concentration of support and catalysts

Catalyst	Acid concentration ($mmol/g_{cat}$)
HBEA	0.84
Ni/BEA-IWI	0.60
Ni/BEA-OR-PH	0.78
Ni/BEA-DP	0.52

The acid concentrations of reduced catalysts in the range of 150~500 °C were determined by quantifying the desorbed NH_3 with NH_3-TPD.
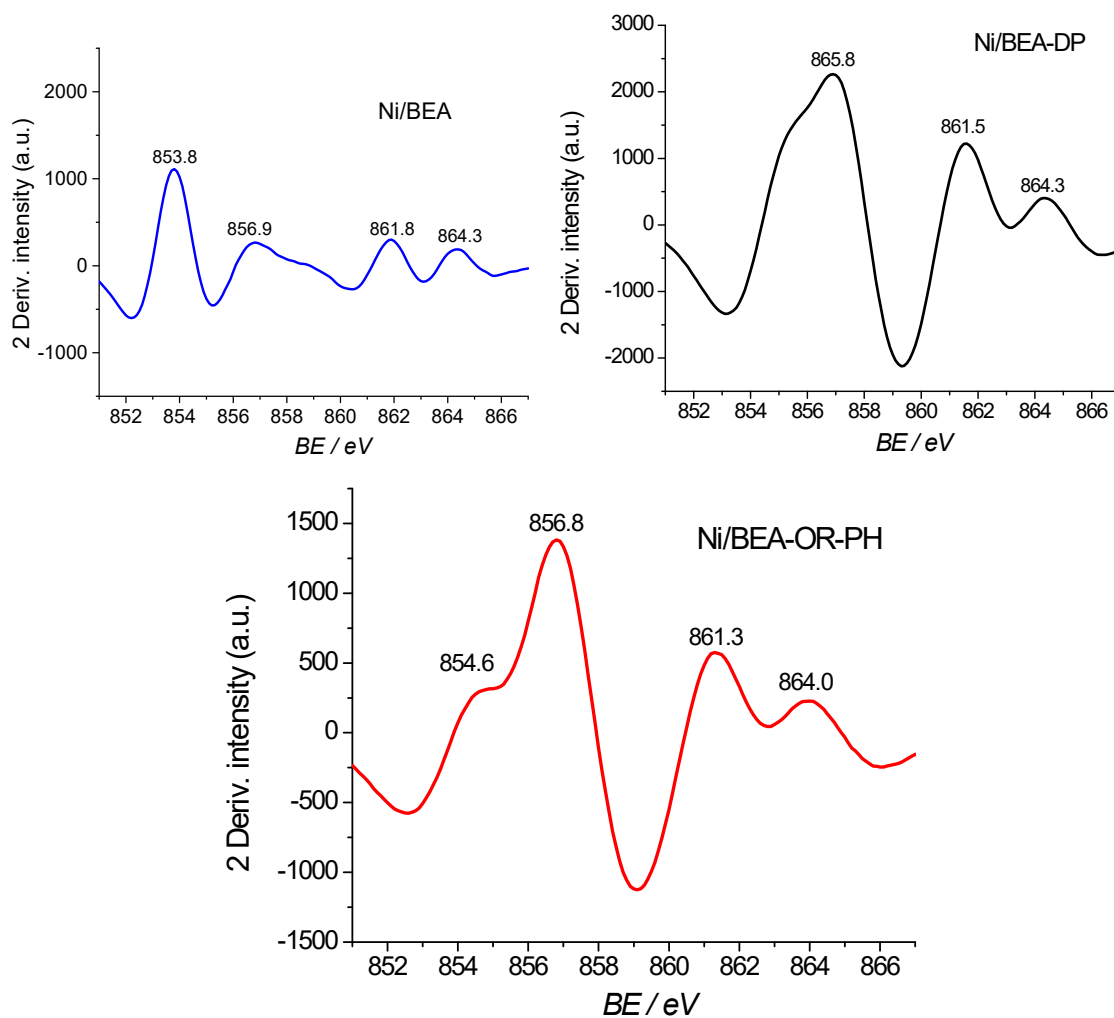

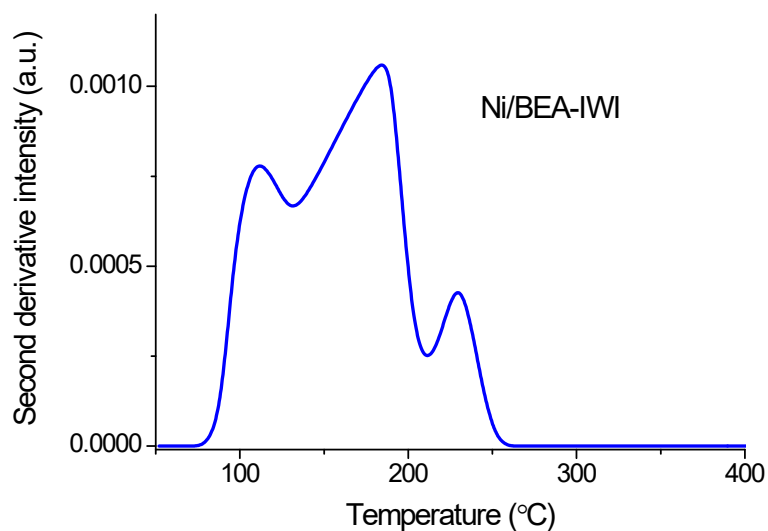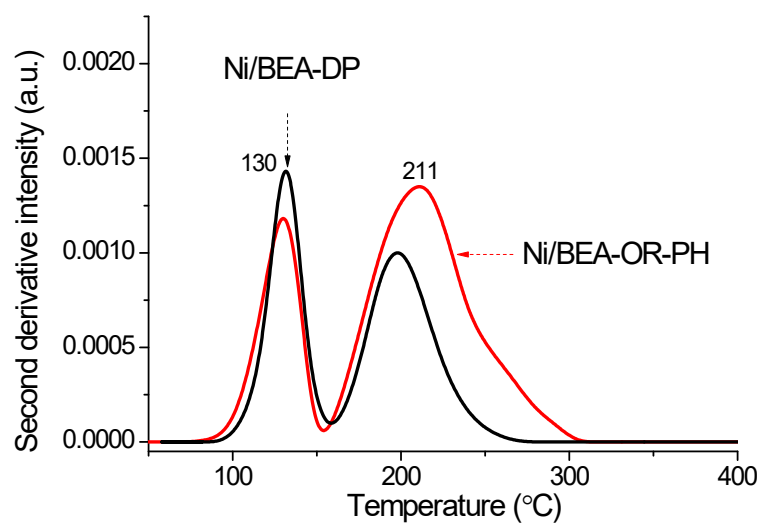**Figure S2**. Second derivative XPS profiles of Ni/BEA catalysts

Figure S3. Second derivative H_2-TPD profiles of pre-reduced Ni/BEA-DP, Ni/BEA-OR-PH and Ni/BEA-IWI catalysts

Table S2. Peak area of low-temperature and high-temperature desorbed H_2

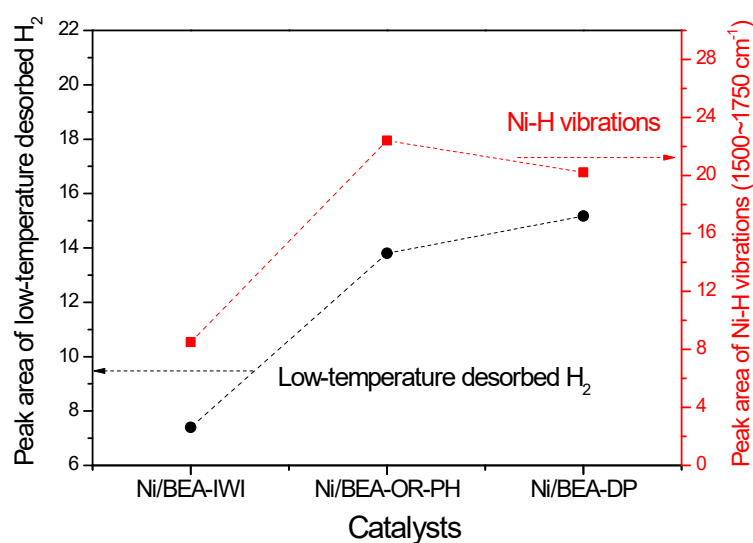| Catalyst	Low-temperature desorbed H_2	high-temperature desorbed H_2
Ni/BEA-IWI	7.66	106.0
Ni/BEA-OR-PH	12.6	231.2
Ni/BEA-DP	14.2	123.4

Figure S4. Relationship of low-temperature desorbed H_2 and Ni-H vibrations

Table S3. HDO of anisole over HBEA

Time (min)	X-$_{anisole}$ (%)	Y-$_{methylansiole}$ (%)	Y-$_{phenol}$ (%)	Y-$_{cresol}$ (%)	Y-$_{guaiacol}$ (%)	Y-$_{1,2-dimethoxy-benezene}$ (%)
0~20	21.1	8.6	6.1	2.6	1.8	1.3
20~40	16.8	6.2	4.8	1.6	3.2	0.6
40~60	12.8	5.1	2.9	0.5	3.2	0

[a] Reaction conditions: WHSV= 2.8 min^{-1}, P(H$_2$) = 4.0 MPa, H$_2$ flow rate=120 mL/min, T=230 °C.

Table S4. TPD of phenol and anisole

Adsorption T (°C)	Desorbed anisole (a.u)	Desorbed phenol (a.u.)	T$_{max-anisole}$[a] (K)	$\Delta E_{des-anisole}$[b] (kJ mol^{-1})	T$_{max-phenol}$[a] (K)	$\Delta E_{des-anisole}$[b] (kJ mol^{-1})
150	2.23	5.43	615	155	632	160
230	0.75	4.06	619	156	626	158
Peak area loss (%)	66%	25%	-	-	-	-

[a] Temperature at peak maxima of desorption from TPD of anisole and phenol; [b] Heat of desorption according to Redhead [1], $\dfrac{\Delta E_{des}}{RT_{max}} = ln\dfrac{v1T_{max}}{\beta}$ -3.64, v_1=10^{13} s^{-1}

Reference

[1] Redhead, P. A. Thermal Desorption of Gases, *Vacuum*, **1962**,12, 203-211.