

## Boosting Cyclopentanone Selective Production via Tuning Electron Effect Between Pt and NiO in MCM-41 Catalysts from Furfural Hydrogenation-rearrangement

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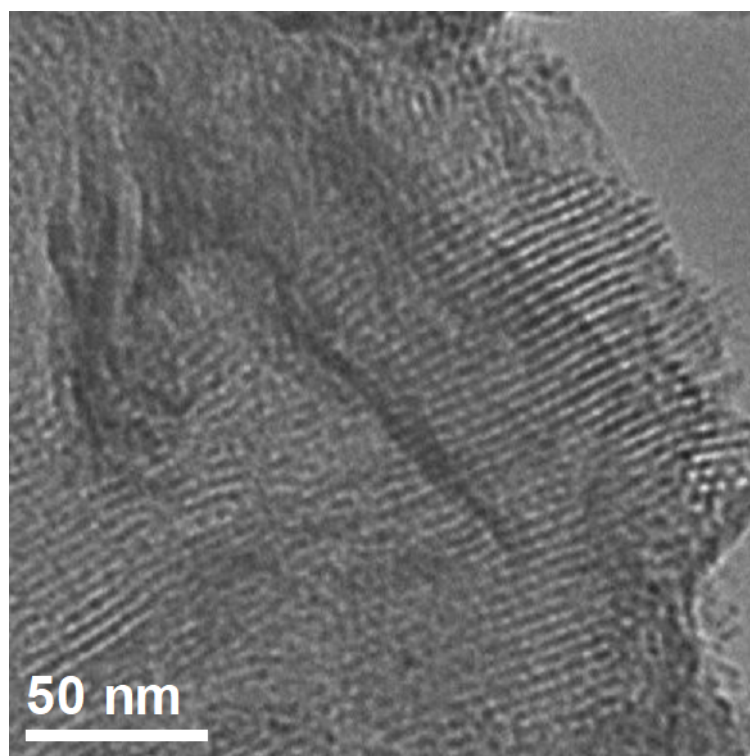


Figure S1 TEM images of 1Pt-3NiO/MCM-41 catalysts

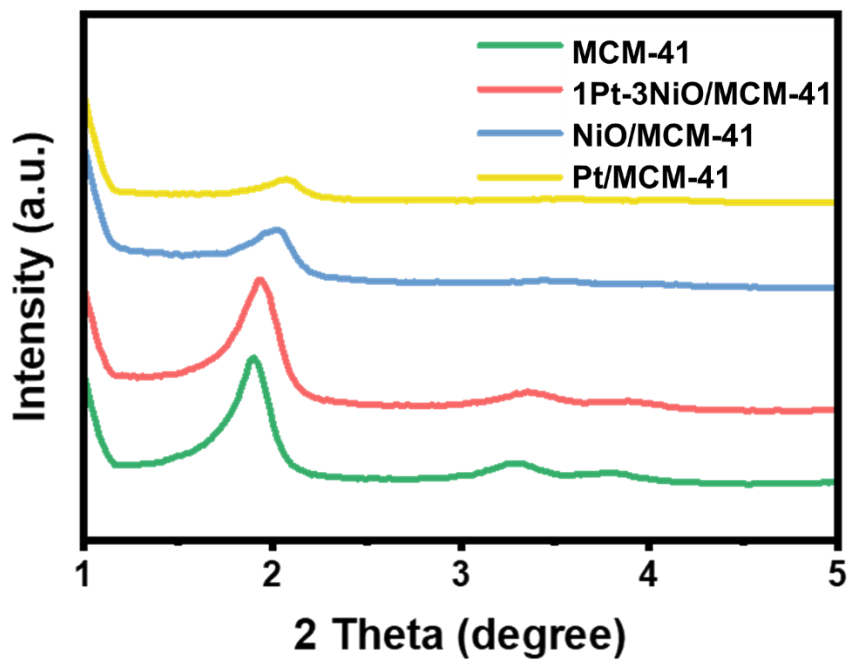


Figure S2 LA-XRD patterns of MCM-41, Pt/MCM-41, NiO/MCM-41 and 1Pt-3NiO/MCM-41 catalysts

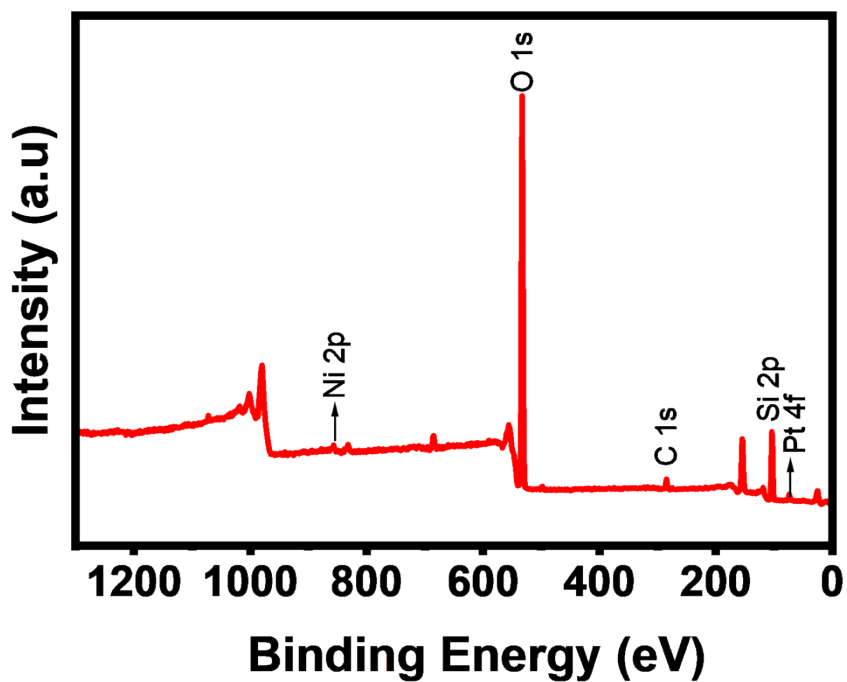


Figure S3 XPS survey spectrum of the 1Pt-3NiO/MCM-41 catalyst

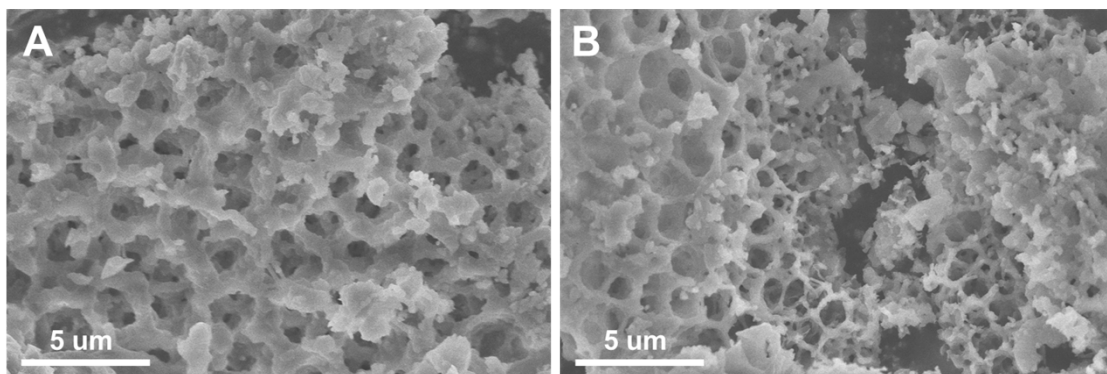


Figure S4 SEM micrographs of the 1Pt-3NiO/MCM-41 catalyst before and after reaction

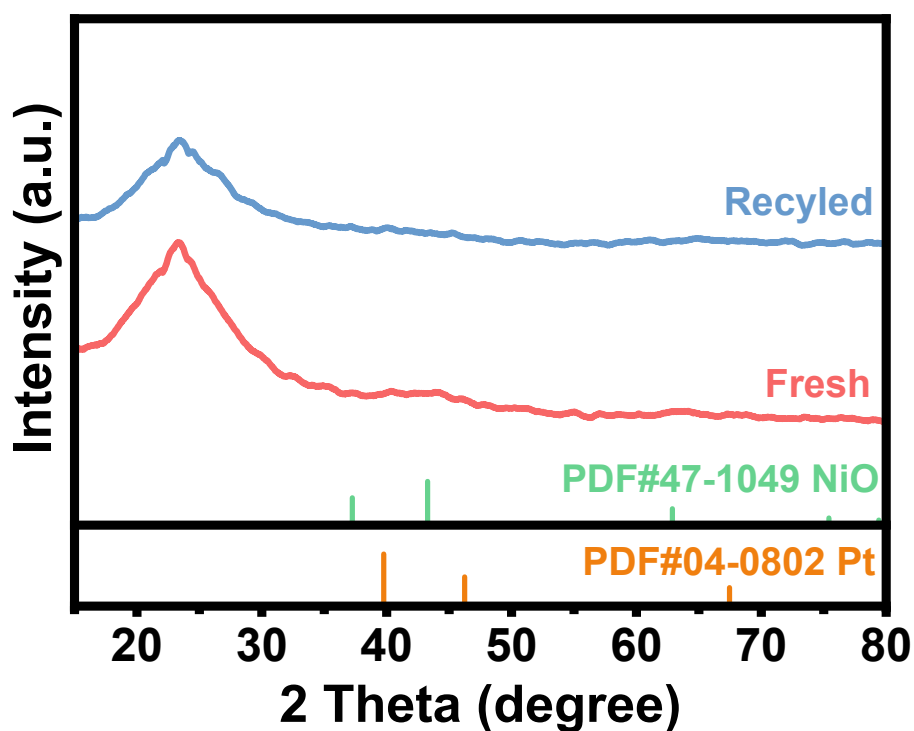


Figure S5 XRD micrographs of the 1Pt-3NiO/MCM-41 catalyst before and after reaction

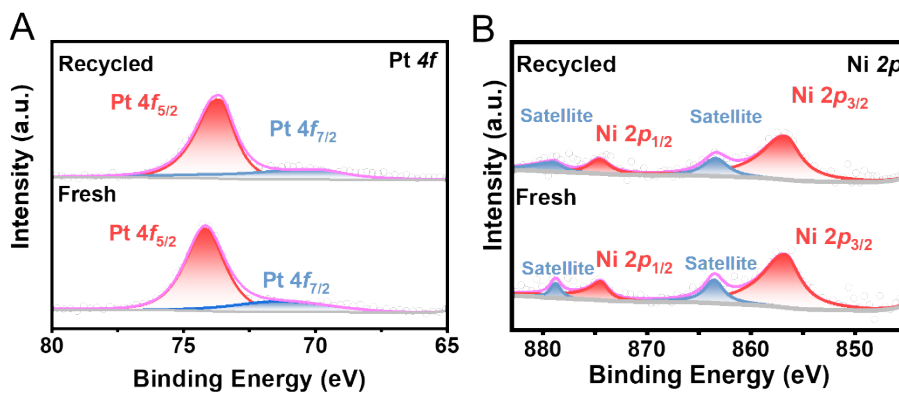


Figure S6 XPS micrographs of the 1Pt-3NiO/MCM-41 catalyst before and after reaction

**Table S1 Elemental analysis of fresh and spent 1Pt-3NiO/MCM-41 samples**

Sample	Pt (wt%)
Fresh catalyst	1.10
Spent catalyst	1.06
Liquid product	0.00

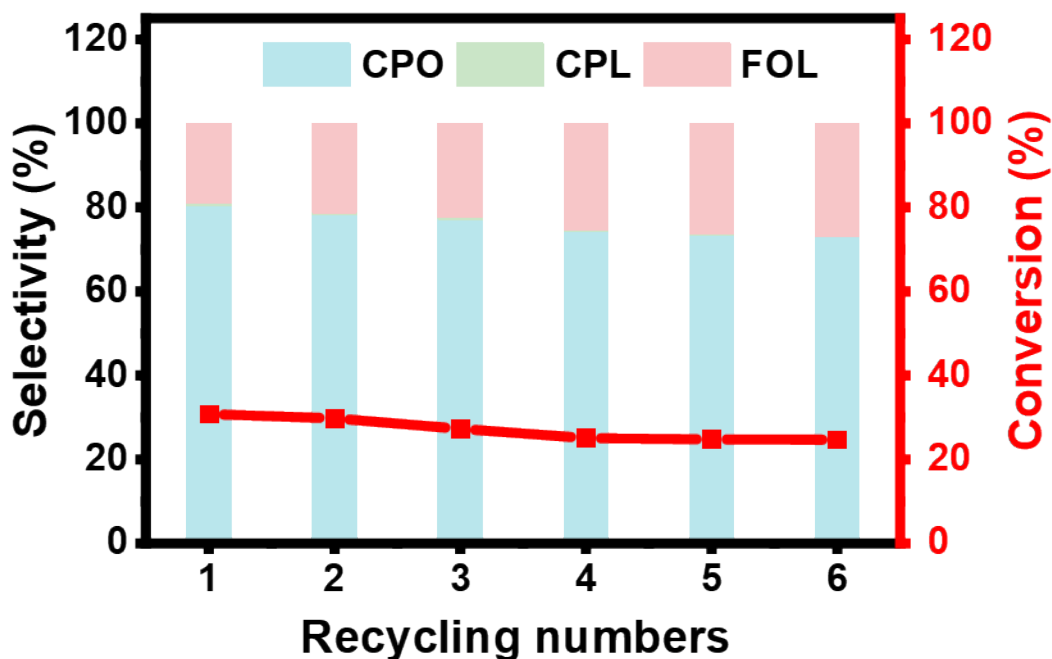


Figure S7 Recyclability of 1Pt-3NiO/MCM-41 catalyst in FAL hydrogenation-rearrangement. The reaction was performed in 20 ml of water containing 83  $\mu$ L of FAL and 10 mg of 1Pt-3NiO/MCM-41 catalysts at 140°C, 2 MPa for 1 h.

After six consecutive recycling tests, the conversion rate of furfural only decreased slightly from approximately 30% to around 25% before stabilizing, indicating that under kinetic limitation conditions, the catalytic activity is well maintained. More importantly, throughout the entire cycling process, the selectivity for the target product CPO remained at a high level with only negligible fluctuations, while the selectivity for the intermediate product FOL and the over-hydrogenation product CPL stayed at a low and stable level. These results strongly confirm that the 1Pt-3NiO/MCM-41 catalyst possesses excellent intrinsic structure and outstanding catalytic stability.

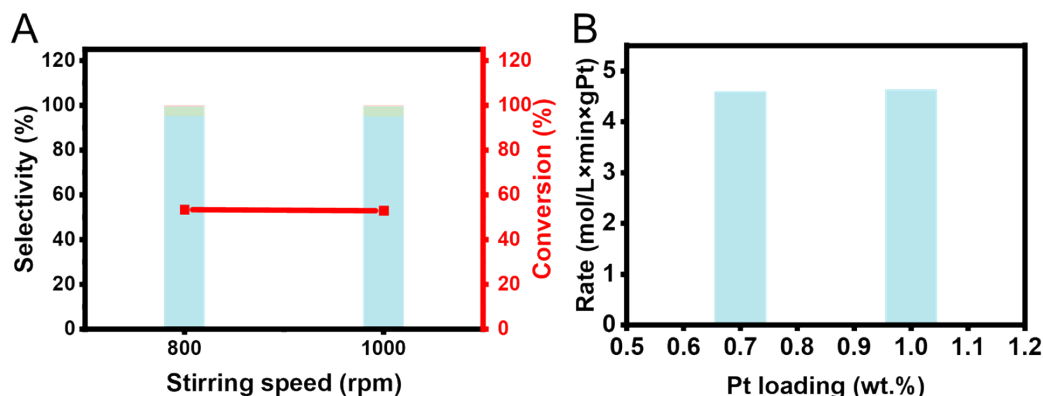


Figure S8 Effects of (A) the stirring speed and (B) Pt loading on the furfural hydrogenation over Pt/MCM-41 (The reaction was performed in 20 ml of water containing 83  $\mu$ L of FAL and 10 mg of Pt/MCM-41 catalysts at 200°C, 2 MPa for 1 h.).

The TOF values were calculated using the following equations:

$$\text{TOF} = \frac{n_{\text{converted FAL}}}{\text{time} \times n_{\text{active atom}}} \times 100\%$$

where  $n_{\text{converted FAL}}$  is the molar amount of FAL converted to the target product CPO, time is the reaction duration, and  $n_{\text{active atom}}$  is the molar amount of surface-active metal atoms rather than total metal atoms. The number of active atoms was

$$n_{\text{active atom}} = \frac{D \times m_{\text{cat}} \times X}{M_{\text{Pt}}} \times 100\%$$

calculated using the formula:

where  $D$  is metal dispersion,  $m_{\text{cat}}$  is catalyst mass,  $X$  is metal loading (wt%), and  $M_{\text{Pt}}$  is the relative atomic mass of Pt. Meanwhile, metal dispersion ( $D_{\text{Pt}}$ ) was determined from the average nanoparticle diameter measured by statistical TEM

analysis using the widely accepted empirical equation:

$$D_{\text{Pt}} = \frac{1.13}{\text{average diameter of Pt}} \times 100\%$$