

Supporting information

Direct synthesis of imines from nitro compounds and biomass-derived carbonyl compounds over nitrogen-doped carbon materials supported Ni nanoparticles

Bo Li, Yanxin Wang, Quan Chi*, Ziliang Yuan, Bing Liu*, and Zehui Zhang*

Key Laboratory of Catalysis and Materials Sciences of Hubei, South-Central University for Nationalities, Wuhan, 430074, China.

*Corresponding author: Tel.: +86-27-67842572. Fax: +86-27-67842572. Bing Liu: E-mail: liubing@mail.scuec.edu.cn; Quan Chi: E-mail: chiquanscuec@163.com

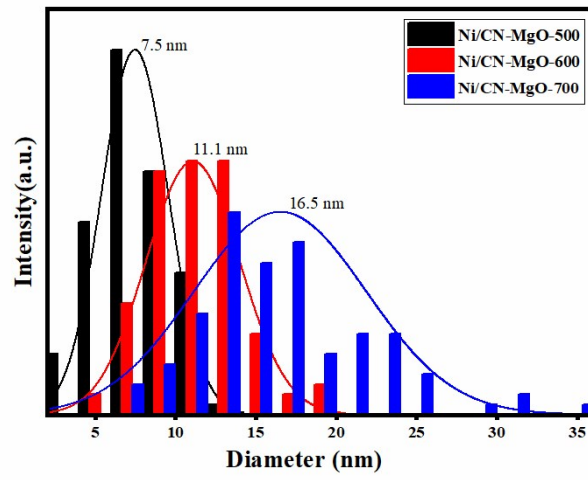
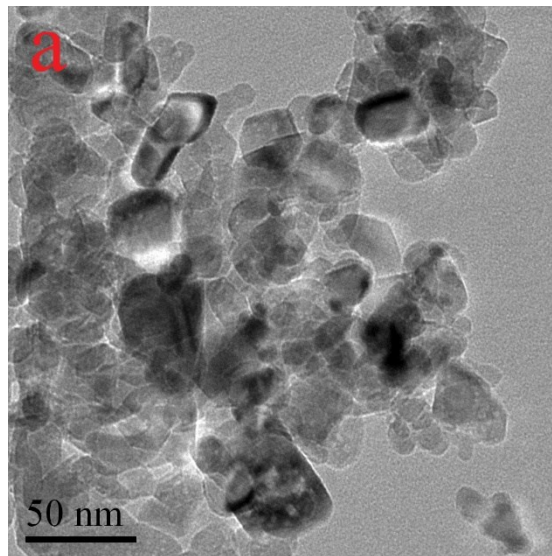


Fig. S1 Particle size distributions for the Ni/CN-MgO-T



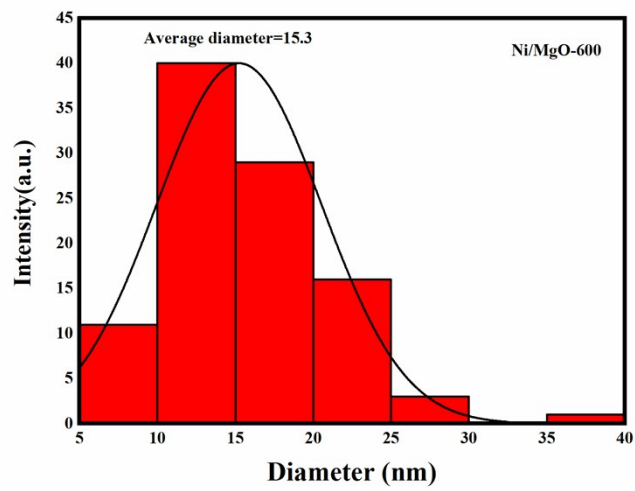
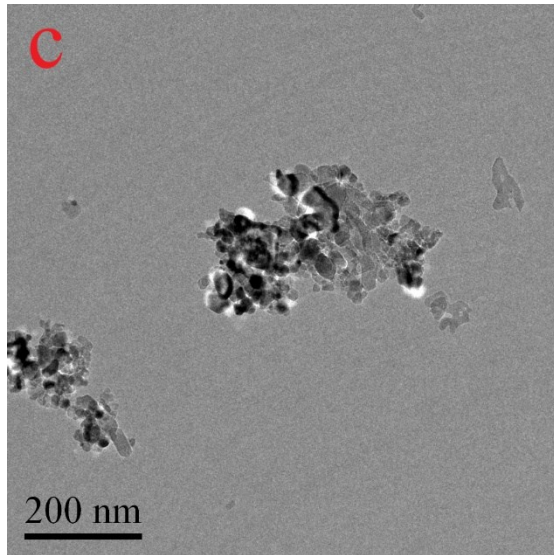
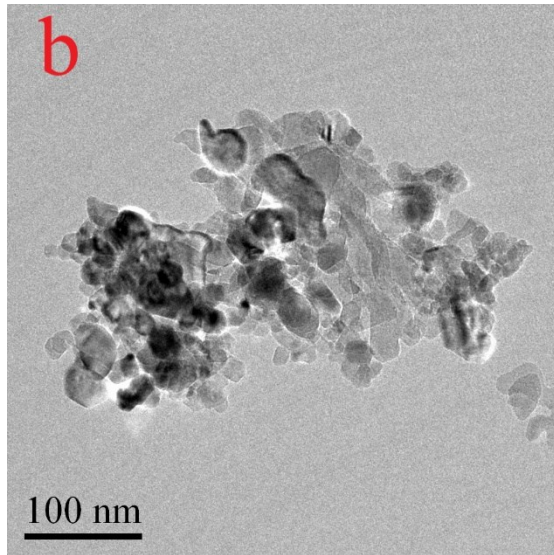


Fig. S2 TEM(a,b,c) and Particle size distributions for the Ni/ MgO-600

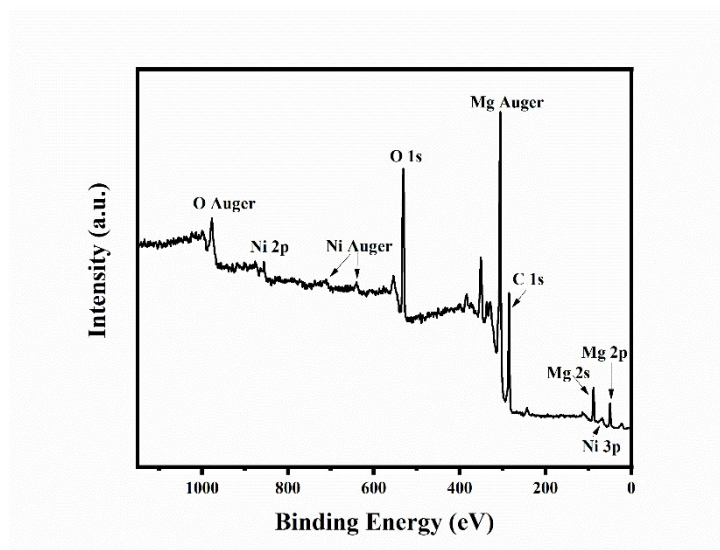


Fig. S3 XPS survey scan of the Ni/CN-MgO-600 catalyst

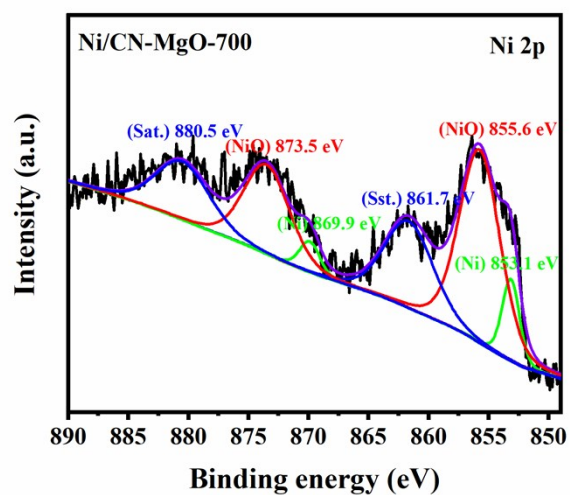
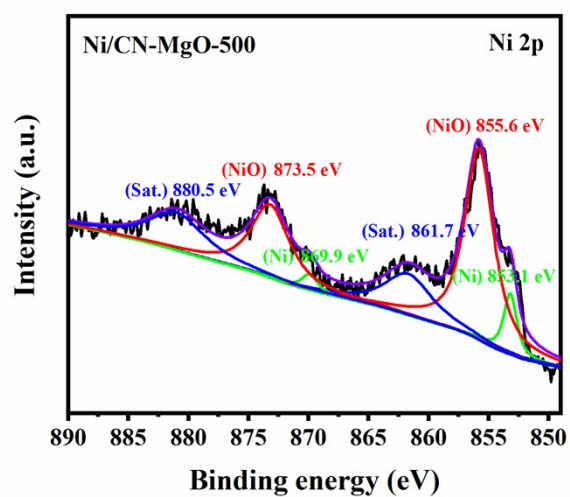


Fig. S4 XPS spectra of Ni 2p in the Ni/NC-MgO-500 and Ni/CN-MgO-700 catalysts

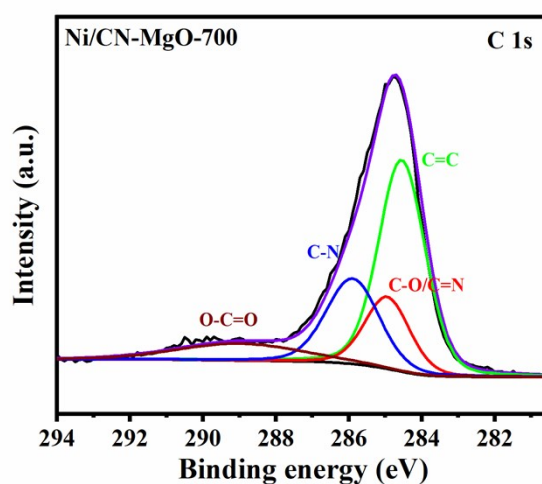
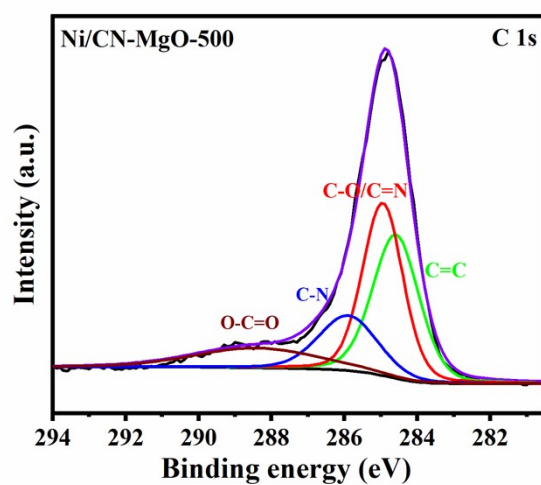


Fig. S5 XPS spectra of C 1s in the Ni/NC-MgO-500 and Ni/CN-MgO-700 catalysts

Table S1. The percentage of different carbon in the Ni/CN-MgO-T catalysts.

| Entry | Samples | O-C=O | C-N | C-O/C=N | C=C |
|-------|---------------|-------|-------|---------|-------|
| 1 | Ni/CN-MgO-500 | 12.7% | 16.7% | 36.0% | 34.6% |
| 2 | Ni/CN-MgO-600 | 11.1% | 19.2% | 29.0% | 40.7% |
| 3 | Ni/CN-MgO-700 | 10.7% | 22.8% | 16.4% | 50.1% |

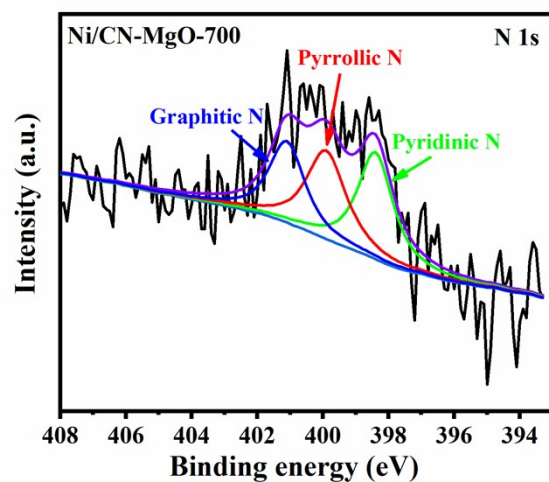
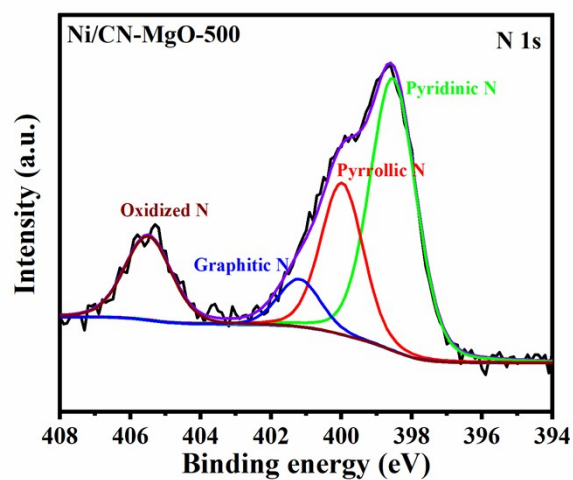


Fig. S6 XPS spectra of N 1s in the Ni/NC-MgO-500 and Ni/CN-MgO-700 catalysts

Table S2. The percentage of different nitrogen in the Ni/CN-MgO-T catalysts

| Entry | Samples | Pyridinic N | Pyrrolic N | Graphitic N | Oxidized N |
|-------|---------------|-------------|------------|-------------|------------|
| 1 | Ni/CN-MgO-500 | 50.4% | 25.7% | 8.2% | 15.7% |
| 2 | Ni/CN-MgO-600 | 49.6% | 32.4% | 18.0% | - |
| 3 | Ni/CN-MgO-700 | 32.2% | 37.6% | 30.2% | - |

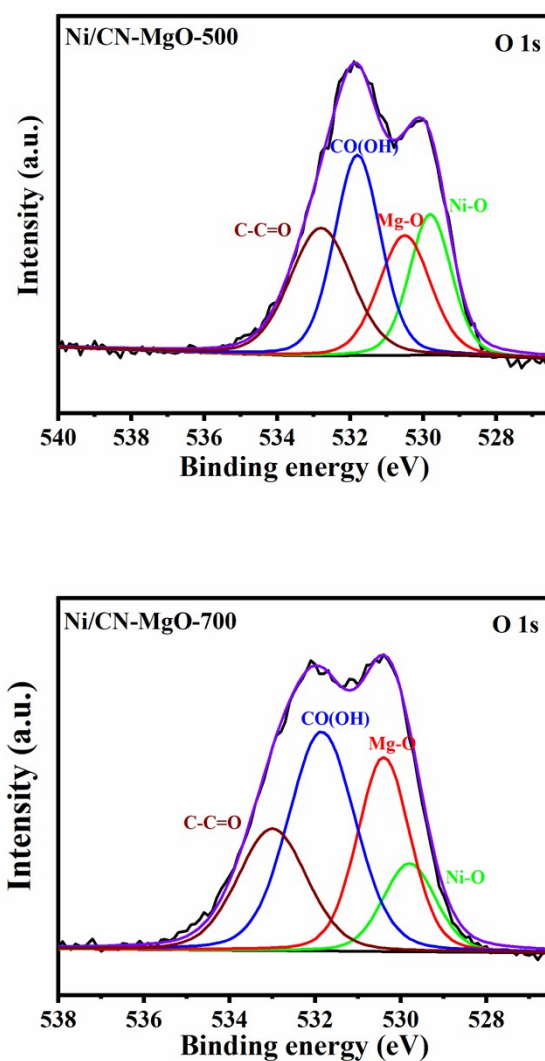


Fig. S7 XPS spectra of O 1s in the Ni/NC-MgO-500 and Ni/CN-MgO-700 catalysts

Table S3. The percentage of different oxygen in the Ni/CN-MgO-T catalysts

| Entry | Samples | Ni-O | Mg-O | CO(OH) | C-C=O |
|-------|---------------|-------|-------|--------|-------|
| 1 | Ni/CN-MgO-500 | 20.1% | 21.1% | 31.8% | 27.0% |
| 2 | Ni/CN-MgO-600 | 16.6% | 22.8% | 35% | 25.6% |
| 3 | Ni/CN-MgO-700 | 12.3% | 26.9% | 38.7% | 22.1% |

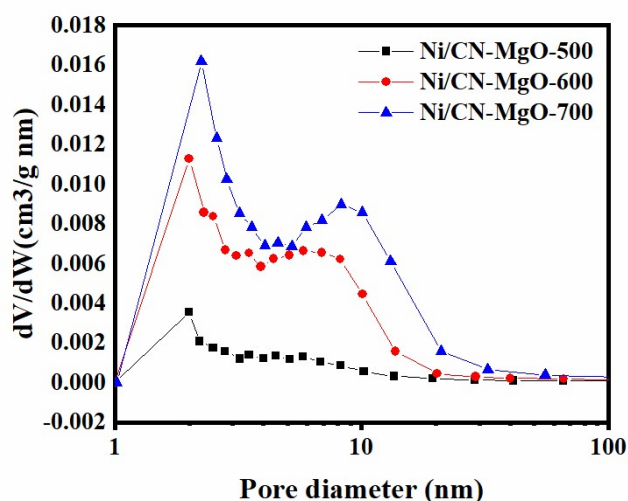


Fig. S8 pore size distributions of the Ni/CN-MgO-T catalysts

Table S4. The texture properties of the as-prepared catalysts.

| Entry | Samples | S_{BET} ($\text{m}^2 \text{g}^{-1}$) | Pore Volume ^a ($\text{cm}^3 \text{g}^{-1}$) | Pore Size ^b (nm) |
|-------|---------------|--|---|--------------------------------|
| 1 | Ni/CN-MgO-500 | 35.5 | 0.039 | 14.0 |
| 2 | Ni/CN-MgO-600 | 181.0 | 0.107 | 7.67 |
| 3 | Ni/CN-MgO-700 | 171.2 | 0.214 | 10.4 |

Table S5. The comparison between other catalysts and our Ni/CN-MgO catalyst.

| Entry | Catalyst | Condition | Compared |
|-------|---|--|---|
| 1 | Au/TiO ₂ ^[1] | 25 °C, 1 mmol H ₂ O, 5 atm CO | The use of precious metals as precursors makes the catalyst expensive. |
| 2 | Au-Pd/Al ₂ O ₃ ^[2] | 140 °C, 2 MPa Ar, 40 mL methanol, 10 mL H ₂ O, 0.5 g cat | The use of precious metals to prepare the catalyst increases the cost of the catalyst. It is also a bimetallic catalyst. At the same time, the temperature condition of the reaction is also harsh. |
| 3 | CoOx@NC-800 ^[3] | 110 °C, 5.0 MPa H ₂ , THF (3.2 mL), H ₂ O (0.8 mL), 24 h | The reaction conditions are harsh such as temperature and pressure. |
| 4 | CoS ₂ @MoS ₂ ^[4] | 60 °C, 1.5 MPa H ₂ | This reaction condition is indeed in compliance with environmental protection regulations, but its poor selectivity makes the |

| | | | |
|---|---|--|--|
| | | | separation work cost much. |
| 5 | PtCo/CoBO _x ^[5] | 60 °C and 1 MPa H ₂ , 5mg Cat | The catalyst is prepared by using precious metals, and it is also a bimetallic catalyst, which is more complicated to prepare. |
| 6 | Ni ₂ Si/SiCN-1000 ^[6] | 170 °C, 5 MPa H ₂ , 100 mg cat | The reaction conditions are very harsh such as reaction temperature and pressure. |
| 7 | Ni/SiO ₂ ^[7] | 378 K, 1.4 MPa H ₂ , 15 mg cat | The preparation method of the catalyst is complicated. |
| 8 | Ni/SiO ₂ ^[8] | 80 °C, 1.4 MPa H ₂ , 5 mg cat | The preparation method of the catalyst is complicated. |
| 9 | Ni/CN-MgO-600 | 80 °C, 1.0 MPa H ₂ , 20 mg cat. | Simple preparation method, economical source of materials. |

[1] J. Huang, L. Yu, L. He, Y. Liu, Y. Cao, K. Fan, *Green Chem.*, 2011, **13**, 2672-2677.

[2] Y. Xiang, Q. Meng, X. Li, J. Wang, *Chem. Commun.*, 2010, **46**, 5918–5920.

[3] T. Song, P. Ren, Y. Duan, Z. Wang, X. Chena, Y. Yang, *Green Chem.*, 2018, **20**, 4629-4637.

[4] W. Han, J. Wang, X. Lia, L. Zhou, Y. Yang, M. Tang, H. Ge, *Catal. Commun.*, 2019, **124**, 86-91.

[5] S. Zhang, Z. Xia, Y. Ma, J. Li, Y. Qu, *J. Catal.*, 2019, **374**, 72-81.

[6] X. Chen, S. Han, D. Yin, C. Liang, *Inorg. Chem. Front.*, 2020, **7**, 82-90.

[7] Y. Zheng, K. Ma, H. Li, J. Li, J. He, X. Sun, R. Li, J. Ma, *Catal. Lett.*, 2009, **128**, 465-474.

[8] B. Li, H. Zeng, *Chem. Mater.*, 2019, **31**, 5320-5330.