Support Information

NH3 production from absorbed NO with synergistic catalysis of Pd/C and functionalized ionic liquids

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Characterization of the IL [TEPA][Im]

The chemical structures of tetraethylenepentamine (TEPA) and imidazole (Im) are shown in Fig. S1.

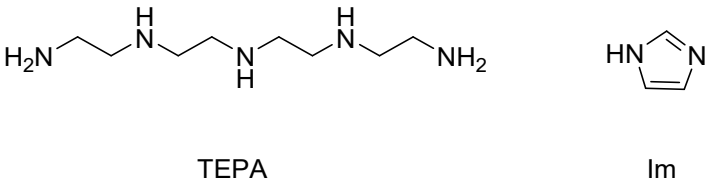

Fig. S1 The chemical structures of tetraethylenepentamine (TEPA) and imidazole (Im).

The structure of the IL [TEPA][Im] was confirmed by ^{1}H NMR, shown in Fig. S2. The attribution of ^{1}H NMR (400 MHz, Chloroform-d) is shown as follows: δ 7.64 (s, 1H), 7.06 (s, 2H), 2.93 – 2.54 (m, 18H), 2.54 – 2.32 (m, 5H).

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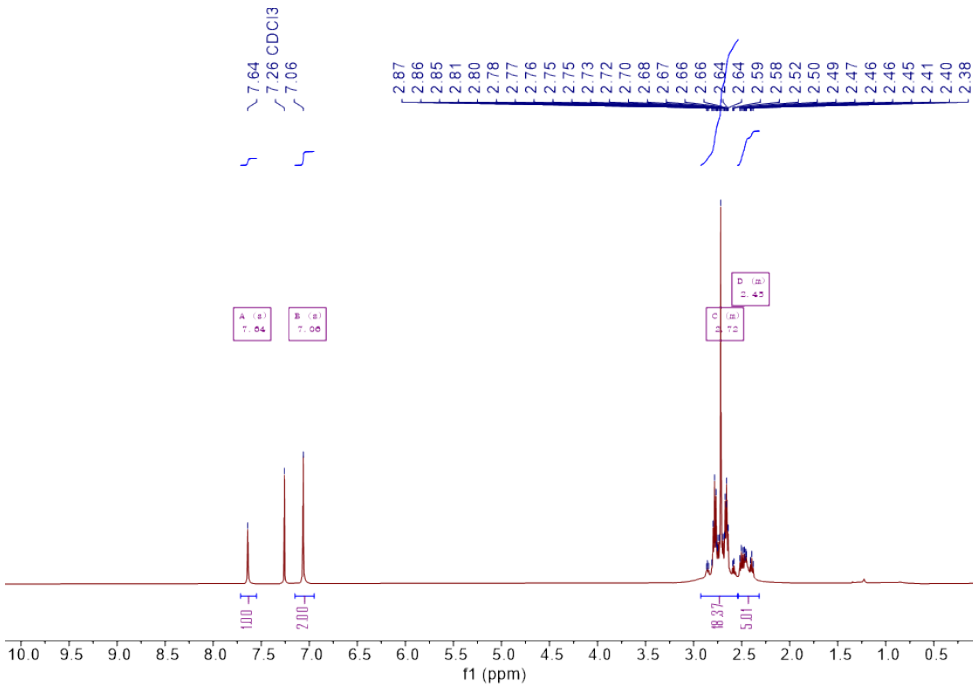


Fig. S2 ^{1}H NMR of [TEPA][Im] synthesized in this work.

The structure of the IL [TEPA][Im] was also confirmed by ^{13}C NMR, shown in Fig. S3. The attribution of ^{13}C NMR (101 MHz, DMSO-d6) is shown as follows: δ 135.66, 122.15, 51.83, 48.59, 40.92.

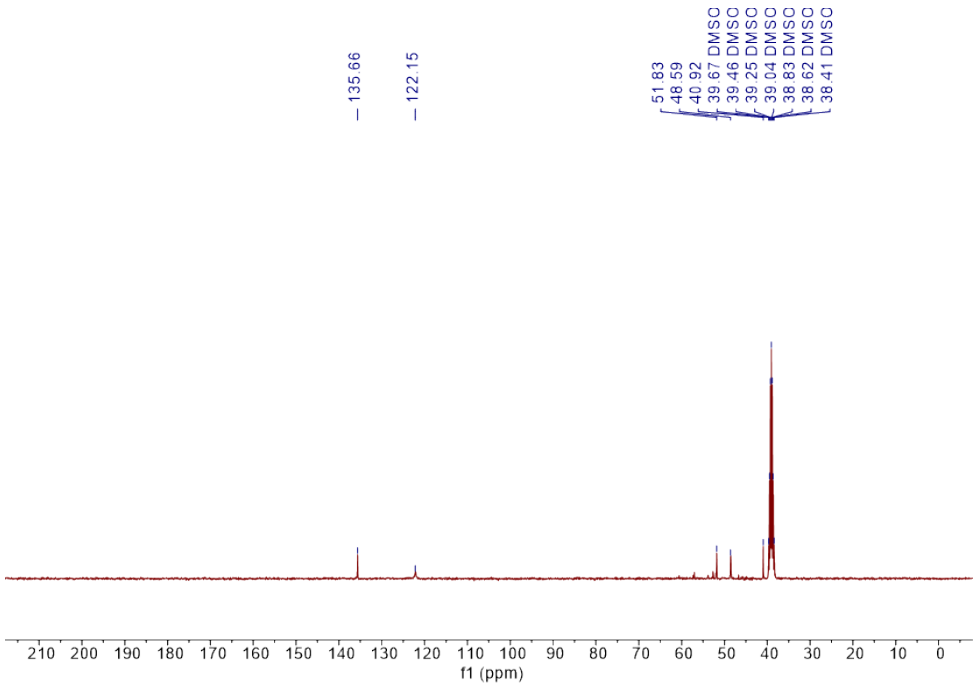


Fig. S3 ^{13}C NMR of [TEPA][Im] synthesized in this work.

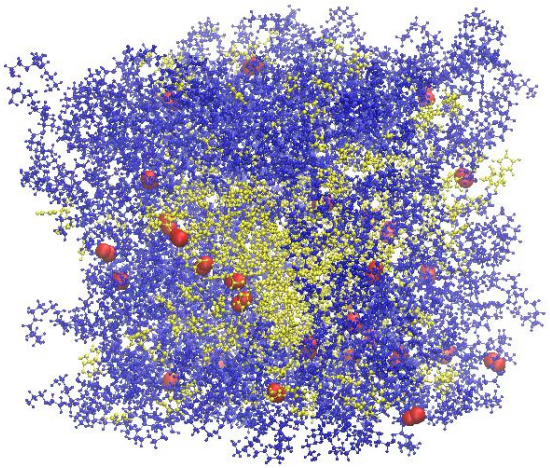


Fig. S4 Snapshot of IL-NO structure at simulation 50 ns.

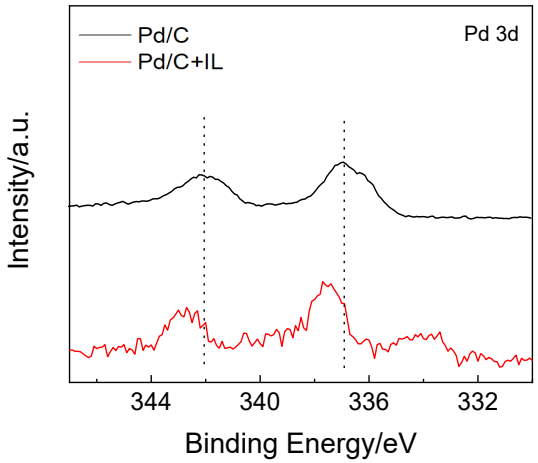
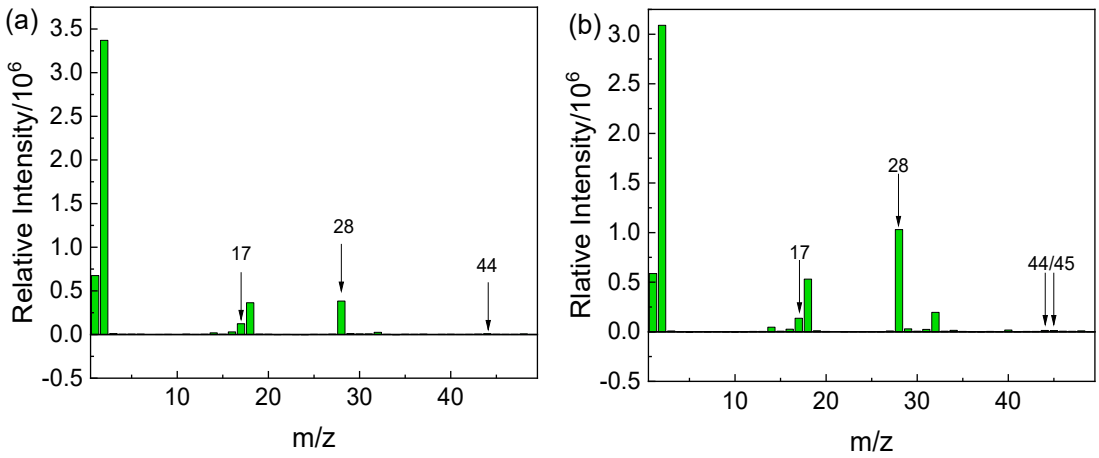


Fig. S5 XPS spectra of Pd/C and Pd/C+IL.



Mass spectrum (m/z): H_2: 1, 2; NH_3: 14, 15, 16, 17; N_2: 14, 28, 29; N_2O: 14, 15, 16, 28, 29, 30, 31, 44, 45.

Fig. S6 Mass spectrometry analysis of reaction products: (a) NO, 0.5 mmol; (b) NO 1.5 mmol. Experimental conditions: [TEPA][Im], 2 g; Pd/C 10 mg; H_2 pressure, 6 MPa; reaction temperature, 100°C; rotational speed, 800 rpm; reaction time, 9 h.

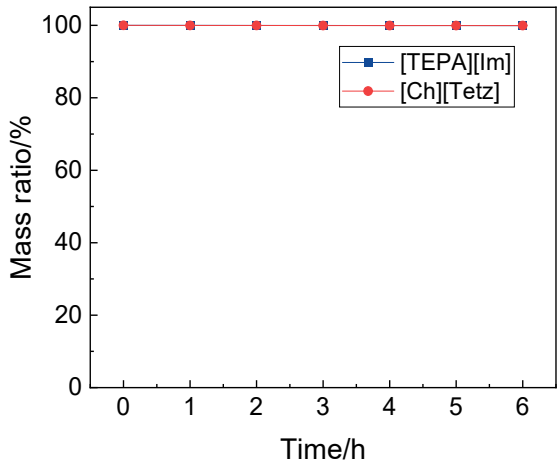


Fig. S7 Thermal stability curve of ionic liquids at 100°C under N_2 (80 mL/min) purge.

Table S1 The yields of N_2 and NH_3 and the conversion of NO under different catalyst dosages and NO contents

Entry	Captured NO/mmol	Catalyst/mg	N_2 yield/%	NH_3 yield/%	NO conversion/%
1	0.5	5	12	37	100
2	0.5	30	34	44	100
3	1.5	20	18	36	100
4	1.5	30	57	25	100

Experimental conditions: [TEPA][Im], 2 g; H_2 pressure, 6 MPa; reaction temperature, 100°C; rotational speed, 800 rpm; reaction time, 9 h.