

## Electronic Supplementary information

### Gold nanoparticles supported on nanoscale amine-functionalized MIL-101(Cr) as a highly active catalyst for epoxidation of styrene

Mrinal Saikia<sup>a,b</sup>, Vasily Kaichev<sup>c</sup> and Lakshi Saikia\*<sup>a,b</sup>

<sup>a</sup>Materials Science and Technology Division,  
CSIR-North East Institute of Science and Technology

Jorhat – 785006, Assam, India

<sup>b</sup>Academy of Scientific and Innovative Research, Chennai, India

<sup>c</sup>Surface Science Laboratory, Boreskov Institute of Catalysis,  
Lavrentieva Ave. 5, 630090, Novosibirsk, Russia

\*Corresponding author. Tel.: +91 376 2370 081; fax. +91 376 2370 011

*\*E-mail address:* l.saikia@gmail.com

#### Table of contents

1. Fig S1 UV spectrum of HAuCl<sub>4</sub> before adsorption (blue) and after adsorption (black) on NH<sub>2</sub>-MIL-101(Cr).
2. Fig S2 NH<sub>2</sub>-MIL-101(Cr) for HAuCl<sub>4</sub> absorption (a) NH<sub>2</sub>-MIL-101(Cr) was added to HAuCl<sub>4</sub> solution (centrifuged after 3h) and (b) HAuCl<sub>4</sub> solution.
3. Fig S3 Zeta potential analysis of the support for determining IEP value.
4. Fig S4 CO<sub>2</sub>-TPD profile of NH<sub>2</sub>-MIL-101(Cr)
5. Fig S5 FE-SEM images of (a) NH<sub>2</sub>-MIL-101 (Cr), (b) Fresh Au/NH<sub>2</sub>-MIL-101(Cr) and (C) Recovered Au/NH<sub>2</sub>-MIL-101(Cr)
6. Fig S6 FT-IR Spectra of NH<sub>2</sub>-MIL-101(Cr) (black), Fresh Au/NH<sub>2</sub>-MIL-101(Cr) (red) and recovered Au/NH<sub>2</sub>-MIL-101(Cr) (blue)
7. Fig S7 XPS spectrum of metallic gold nanoparticles supported on NH<sub>2</sub>-MIL-101(Cr)
8. Fig S8 BJH plot of Au/NH<sub>2</sub>-MIL-101(Cr)
9. Fig S9 Thermogravimetric(black) and derivative curve (blue) of Au/NH<sub>2</sub>-MIL-101(Cr)
10. Fig S10 EDS and mapping analysis of the recovered Au/NH<sub>2</sub>-MIL-101(Cr)
11. Fig S11 TEM images of the recovered Au/NH<sub>2</sub>-MIL-101(Cr)
12. Table S1 Effect of reaction time
13. Table S2 Epoxidation of styrene by TBHP in presence of different gold- based catalyst

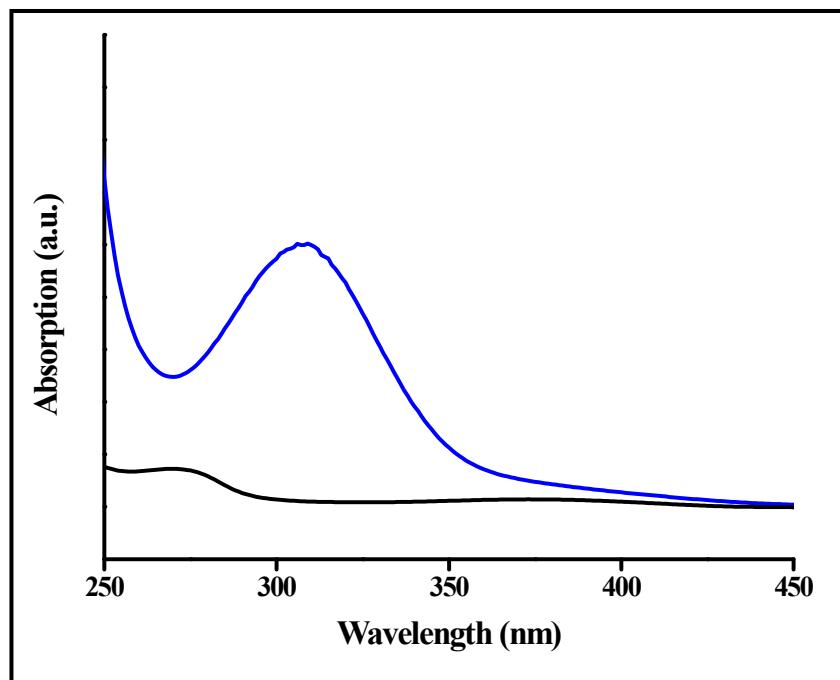


Fig S1 UV spectrum of HAuCl<sub>4</sub> before adsorption (blue) and after adsorption (black) on NH<sub>2</sub>-MIL-101(Cr)

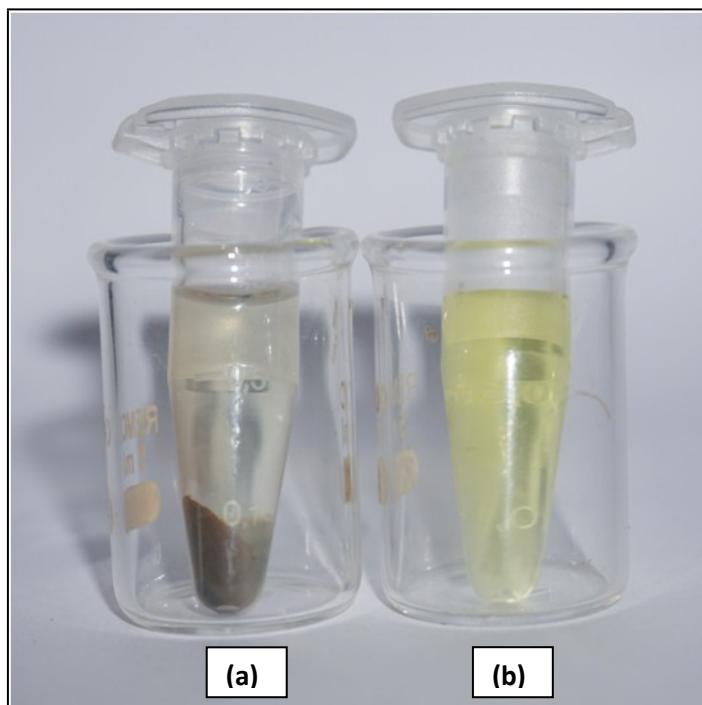


Fig S2 NH<sub>2</sub>-MIL-101(Cr) for HAuCl<sub>4</sub> absorption (a) NH<sub>2</sub>-MIL-101(Cr) was added to HAuCl<sub>4</sub> solution (centrifuged after 3h) and (b) HAuCl<sub>4</sub> solution.

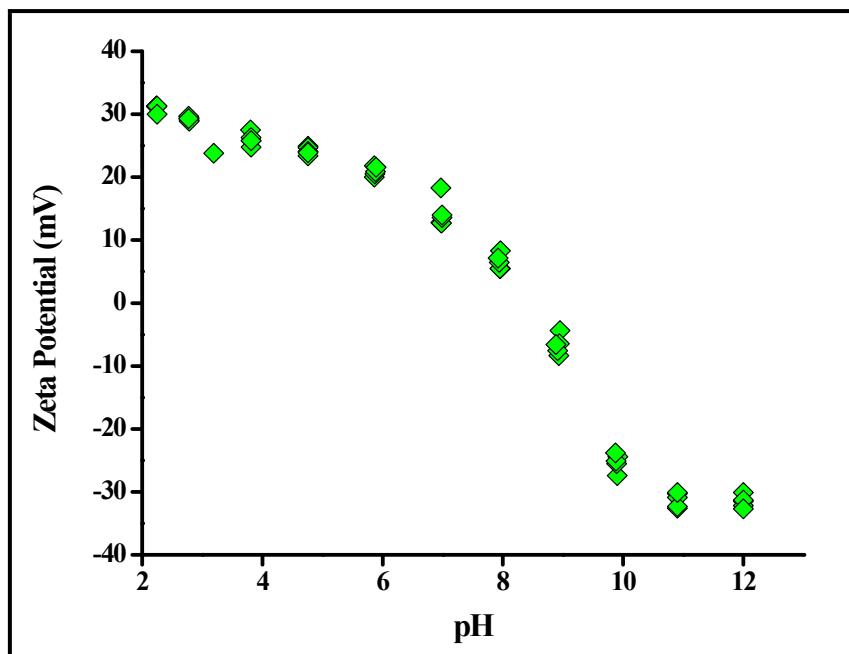


Fig S3 Zeta potential analysis of the support for determining IEP value.

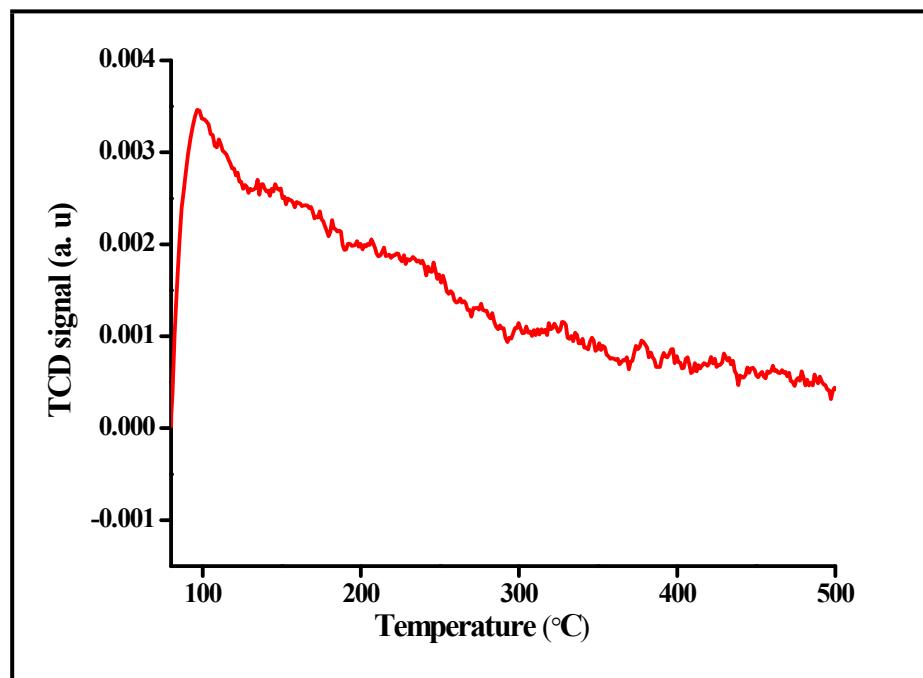


Fig S4 CO<sub>2</sub>-TPD profile of NH<sub>2</sub>-MIL-101(Cr)

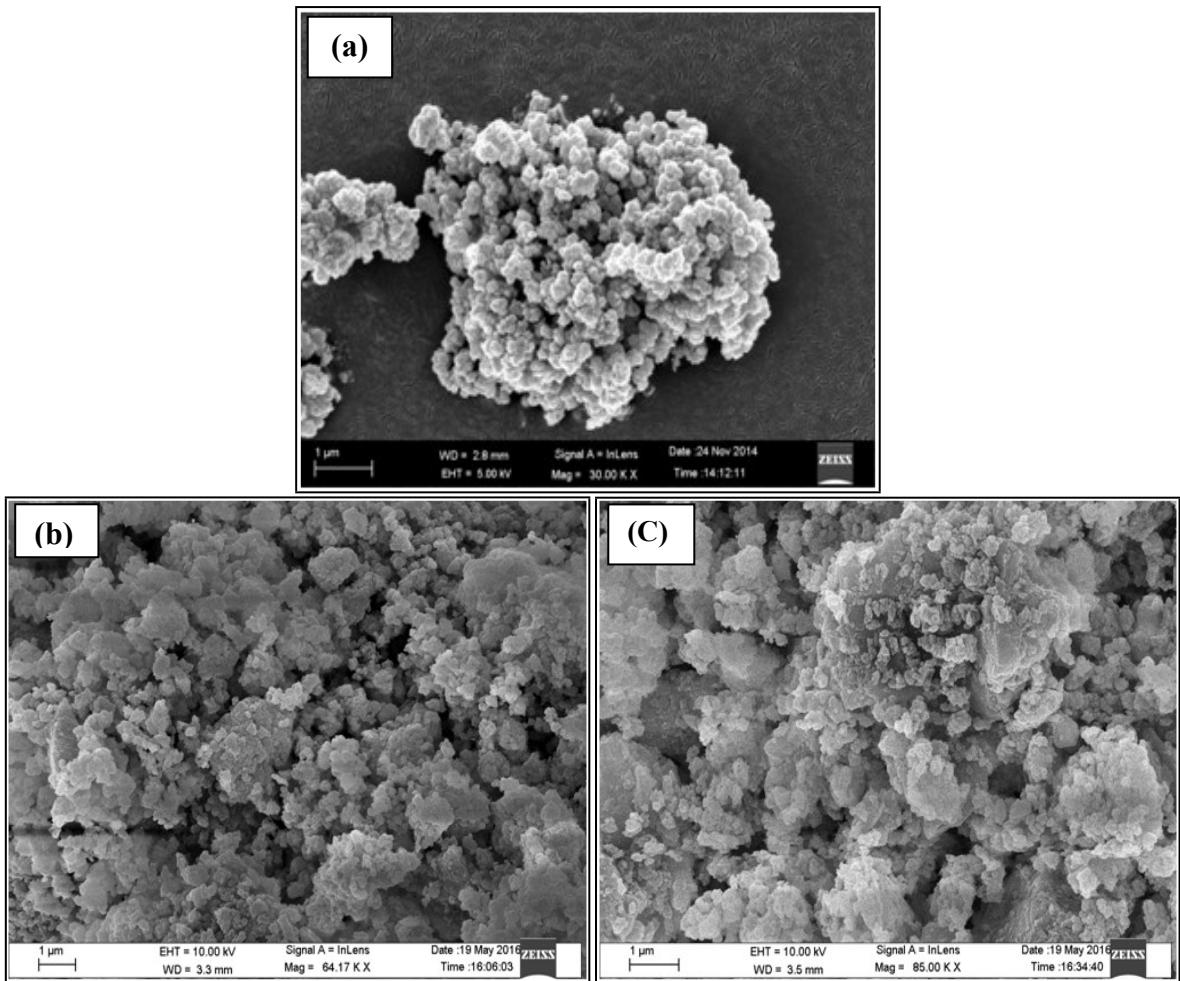


Fig S5 FE-SEM images of (a) NH<sub>2</sub>-MIL-101 (Cr), (b) Fresh Au/NH<sub>2</sub>-MIL-101(Cr) and (C) Recovered Au/NH<sub>2</sub>-MIL-101(Cr)

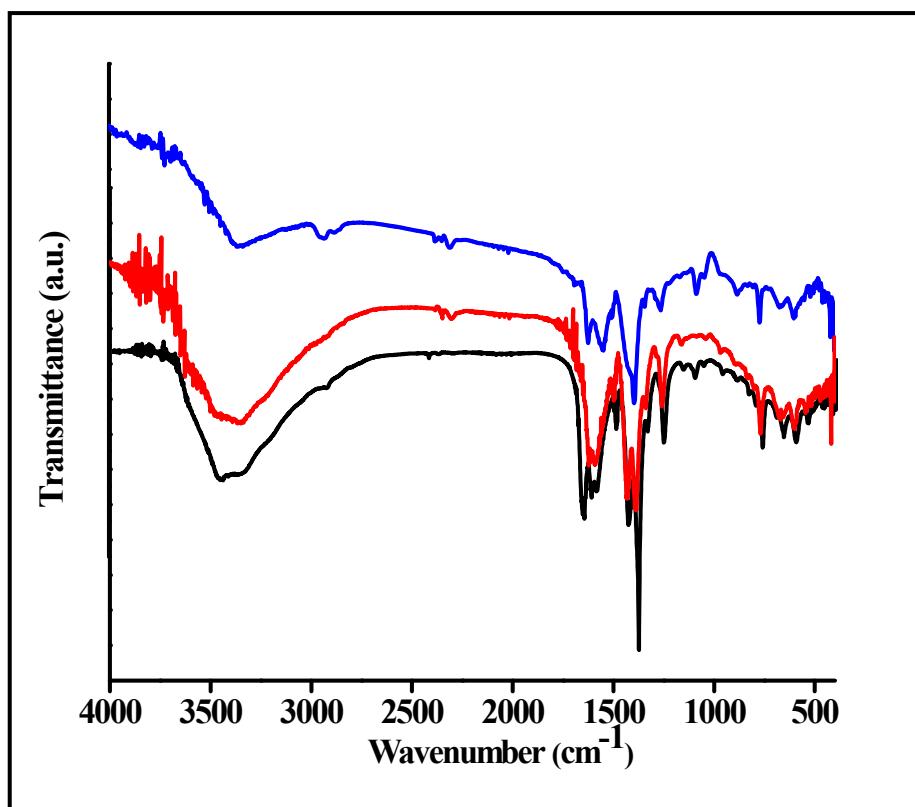


Fig S6 FT-IR Spectra of NH<sub>2</sub>-MIL-101(Cr) (black), Fresh Au/NH<sub>2</sub>-MIL-101(Cr) (red) and recovered Au/NH<sub>2</sub>-MIL-101(Cr) (blue)

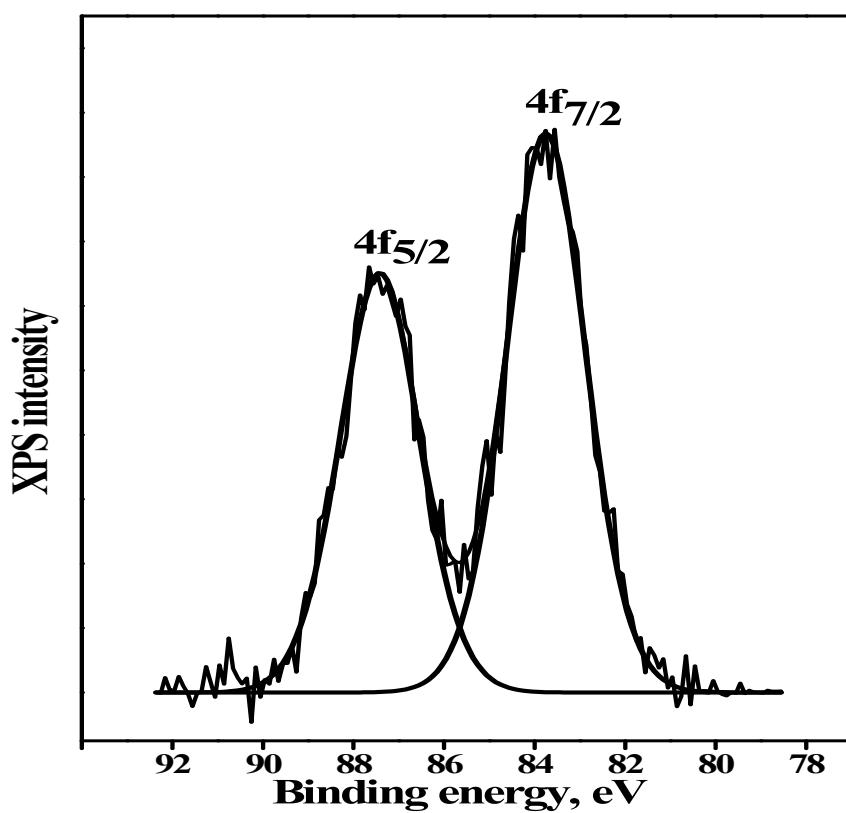


Fig S7 XPS spectrum of metallic gold nanoparticles supported on NH<sub>2</sub>-MIL-101(Cr)

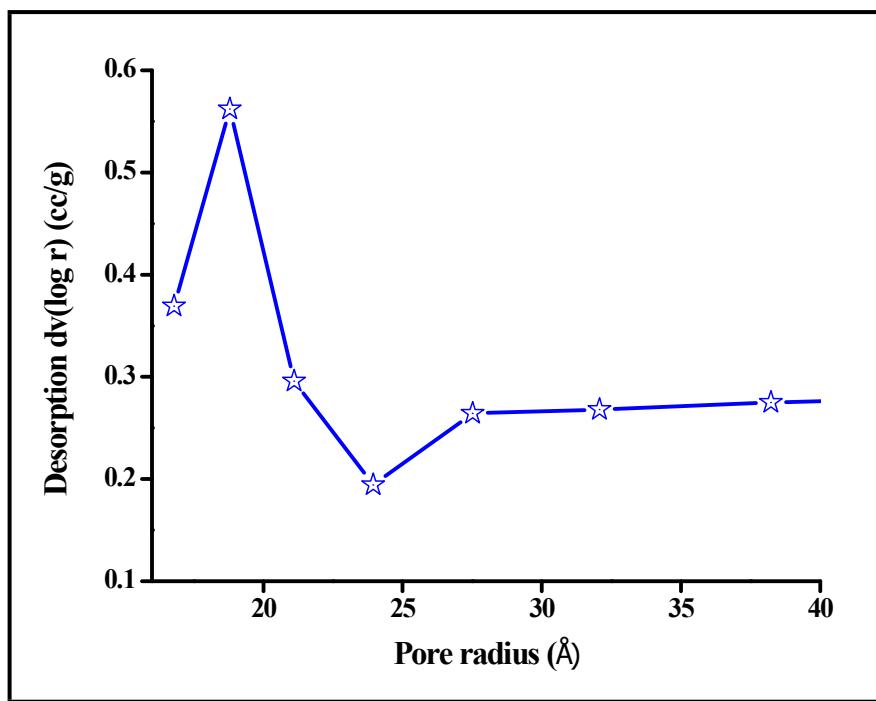


Fig S8 BJH plot of Au/NH<sub>2</sub>-MIL-101(Cr)

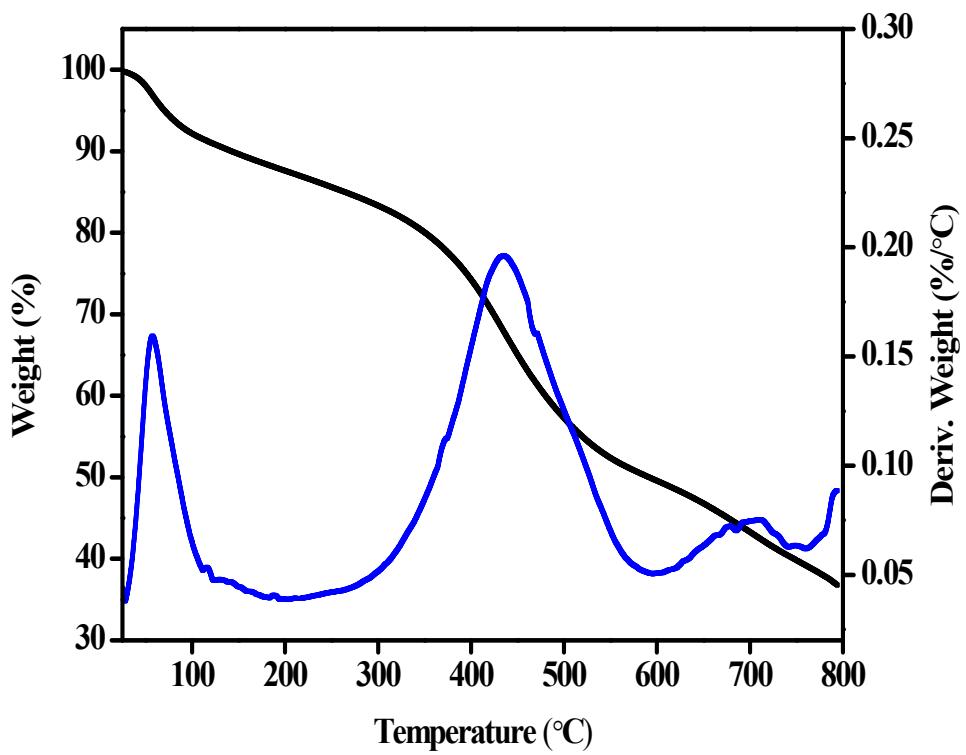


Fig S9 Thermogravimetric (black) and derivative curve (blue) of Au/NH<sub>2</sub>-MIL-101(Cr)

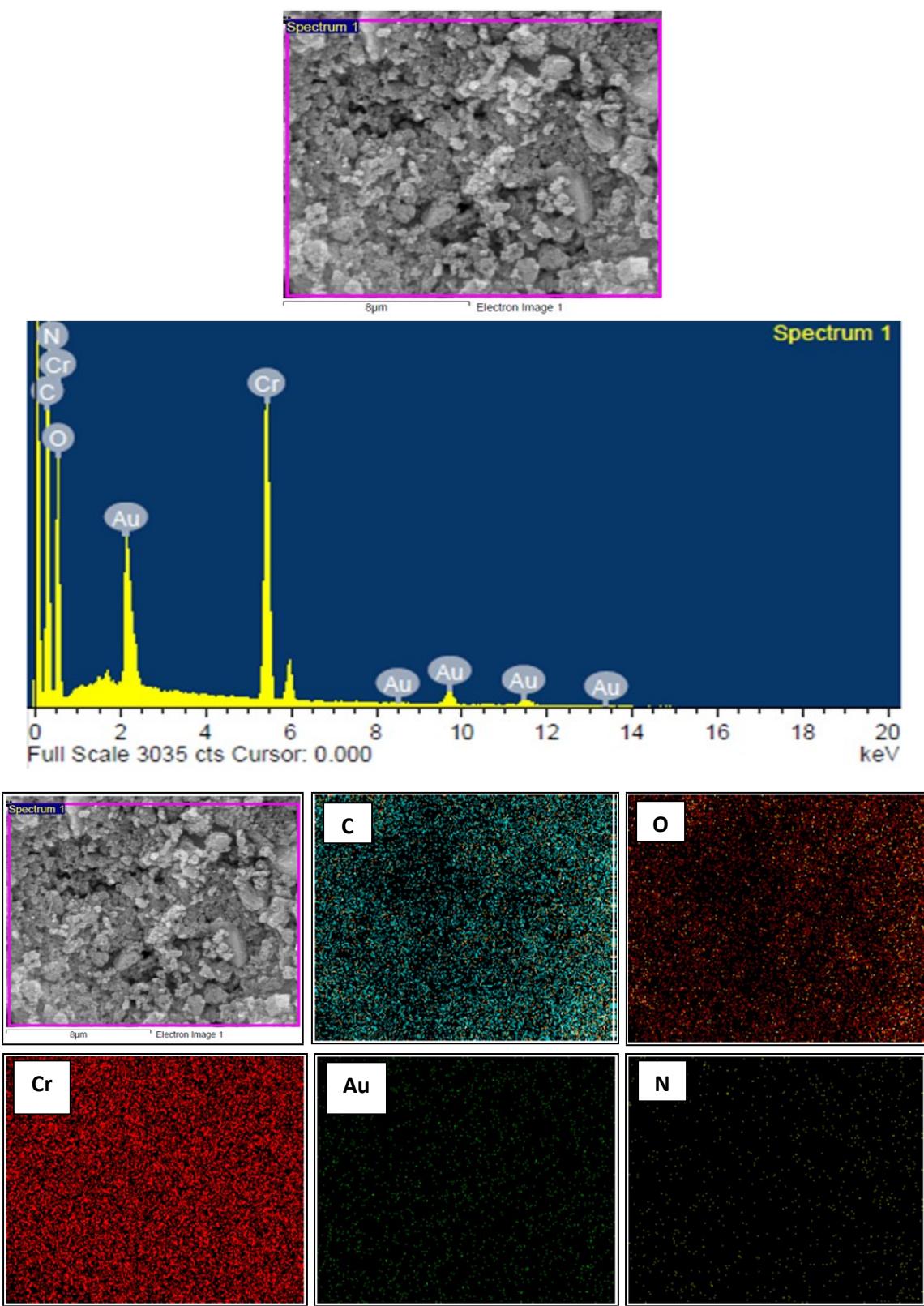


Fig S10 EDS and mapping analysis of the recovered Au/NH<sub>2</sub>-MIL-101(Cr)

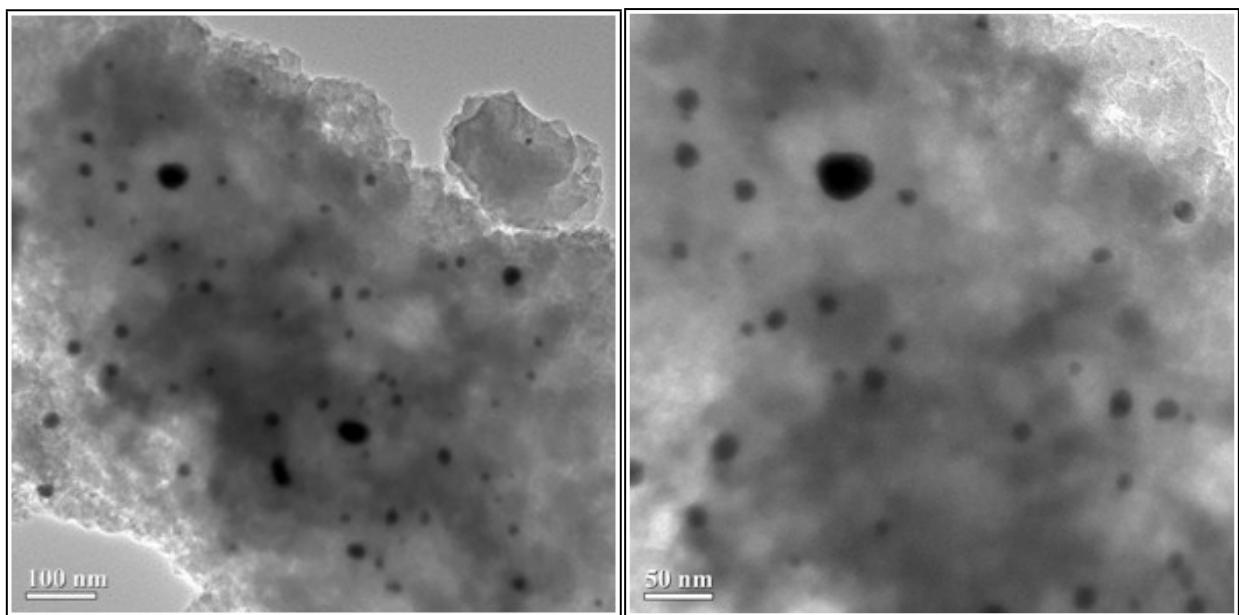


Fig S11 TEM images of the recovered Au/NH<sub>2</sub>-MIL-101(Cr)

Table S1 Effect of reaction time<sup>a</sup>

Entry	Time (h)	Conversion (%)	Selectivity (%)			
			Styrene oxide	Benzaldehyde	Phenylacetaldehyde	Other products
1	4	55.9	84.4	0.0	0.0	15.5
2	8	88.2	74.7	0.0	0.35	24.9
3	12	97.02	19.9	48.3	13.8	17.8

<sup>a</sup>Reaction condition: Styrene (1 mmol), TBHP ( 1.5 mmol), toluene (5 mL), Temperature (110° C), Au/NH<sub>2</sub>-MIL-101(Cr) (0.025 mol%), <sup>b</sup>GC conversion and selectivity

Table S2 Epoxidation of styrene by TBHP in presence of different gold- based catalyst

Entry	Catalysts	Conversion (%)	Selectivity <sup>a</sup> (%)	TOF (mol g <sup>-1</sup> h <sup>-1</sup> ) <sup>c</sup>	Ref.
1	Au/CaO(HDP) <sup>b</sup>	53.6	60.2	0.23	10
2	Au/BaO (HDP)	55.9	53.5	0.19	10
3	Au/SrO (HDP)	53.0	44.8	0.15	10
4	Au/MgO	62.6	54.3	0.28	25
5	Au- <i>meso</i> -Al <sub>2</sub> O <sub>3</sub>	84.3	69.0	0.35	25
6	Au-PMO-SBA-15	94.8	75.0	0.40	25
7	Au/SiO <sub>2</sub>	80.6	38.1	0.28	A
8	GNP/PEG6000-VIC	20.4	62.0	1.32	B
9	Au/Yb <sub>2</sub> O <sub>3</sub> (HDP)	63.5	54.8	0.17	C
10	Au/NH <sub>2</sub> -MIL-101(Cr)	88.2	74.7	1.69	Present Work

<sup>a</sup> Selectivity w.r.t styrene oxide

<sup>b</sup> HDP= homogeneous deposition–precipitation

<sup>c</sup>Turnover frequency (TOF) is calculated by the expression [product]/[Au]×time (h<sup>-1</sup>)

## References

- A. L. Guo, R. Zhang, C. Chen, J. Chen, X. Zhao, A. Chen, X. Liu, Y. Xiu and Z. Hou, *Phys. Chem. Chem. Phys.*, 2015, **17**, 6406.
- B. A. Zeng, Y. Li, S. Su, D. Li, B. Hou and N. Yu, *J. Catal.*, 2014, **319**, 163.
- C. V. R. Choudhary, D. K. Dumbre, N. S. Patil, B. S. Uphade and S. K. Bhargava, *J. Catal.*, 2013, **300**, 217.