Supporting Information

Mesoporous TUD-1 Supported Indium Oxide Nanoparticles for Epoxidation of Styrene using Molecular O_2

Sumbul Rahman,[a] S. A. Farooqui,[b] Aditya Rai,[b] Rawesh Kumar,[a] Chiranjit Santra,[a] Vinod C Prabhakaran,[c] Gopala Ram Bhadu,[d] Debasis Sen,[e] S. Mazumder,[e] Sudip Maity,[f] Anil Sinha*[b] and Biswajit Chowdhury*[a]

GC Analysis details (S1)

Column details and GC condition.

SE-30 Packed column, FID detector, Column length = 8 feet, Oven Temp. 210 °C, Injector and Detector Temp. 230 °C.

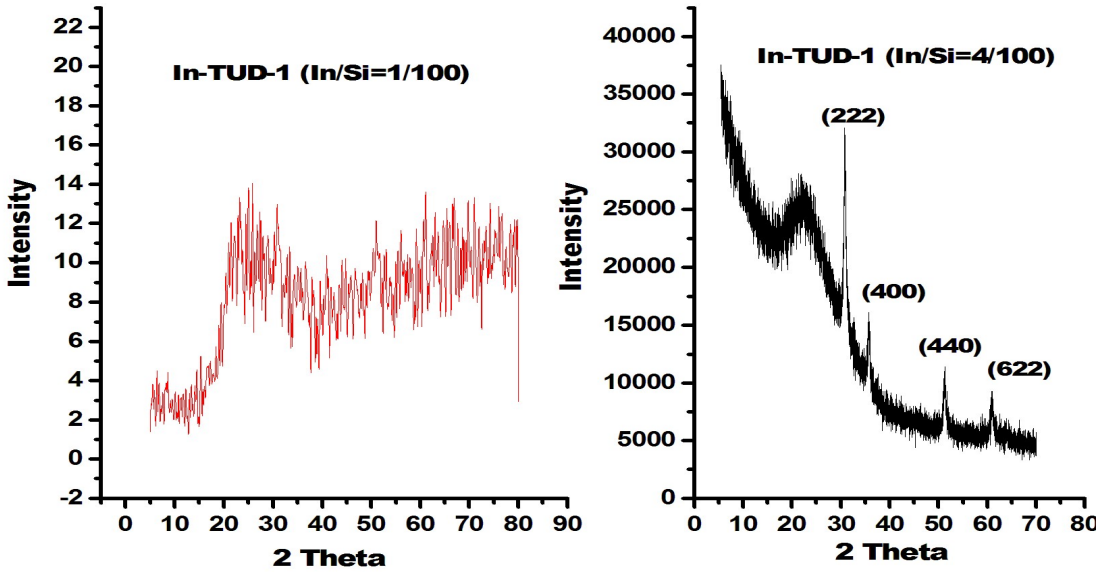

Fig. S2. Diffractograms of In-TUD-1 catalysts with two different loadings.

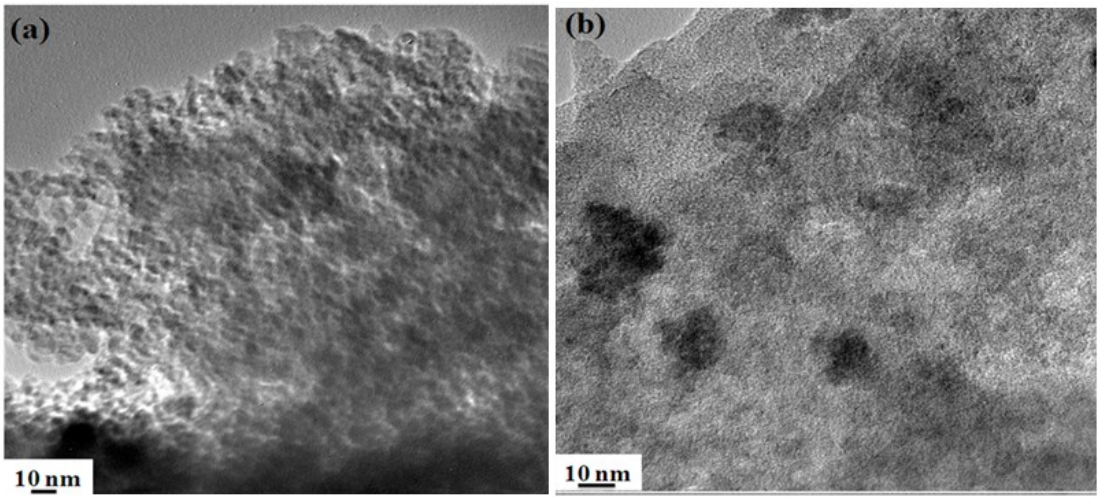

Fig. S3 HRTEM images of In-TUD-1 (a) In/Si = 1/100 and (b) 4/100 catalysts.

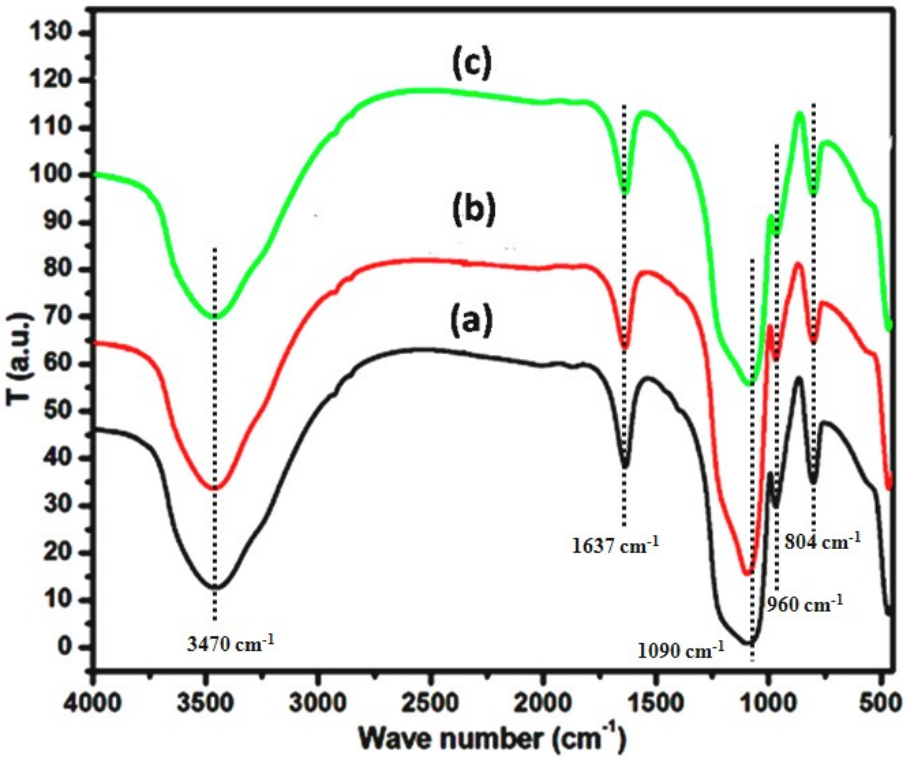

Fig. S4 FTIR spectra of (a) TUD-1 (b) In-TUD-1 (In/Si = 1/100) (c) In-TUD-1 (In/Si = 4/100).

Table S5. Catalytic data for In-TUD-1 (In/Si = 1/100) catalyst for Styrene epoxidation reaction at different solvent.

Catalyst	Solvent	Conversion (%)	Selectivity (%)	
			Styrene Oxide	Benzaldehyde
In-TUD-1	DMF	24.7	57.0	42.9
In-TUD-1	1-4 Dioxane	-	-	-
In-TUD-1	Acetonitrile	-	-	-
In-TUD-1	Decane	-	-	-

Reaction conditions: DMF, 10 mL; Styrene, 6.5 mmol; Dodecane, 0.1 mL; catalyst, 0.1 g; O_2 flow rate, 10 mL min^{-1}, 130 ^oC; 8 h.

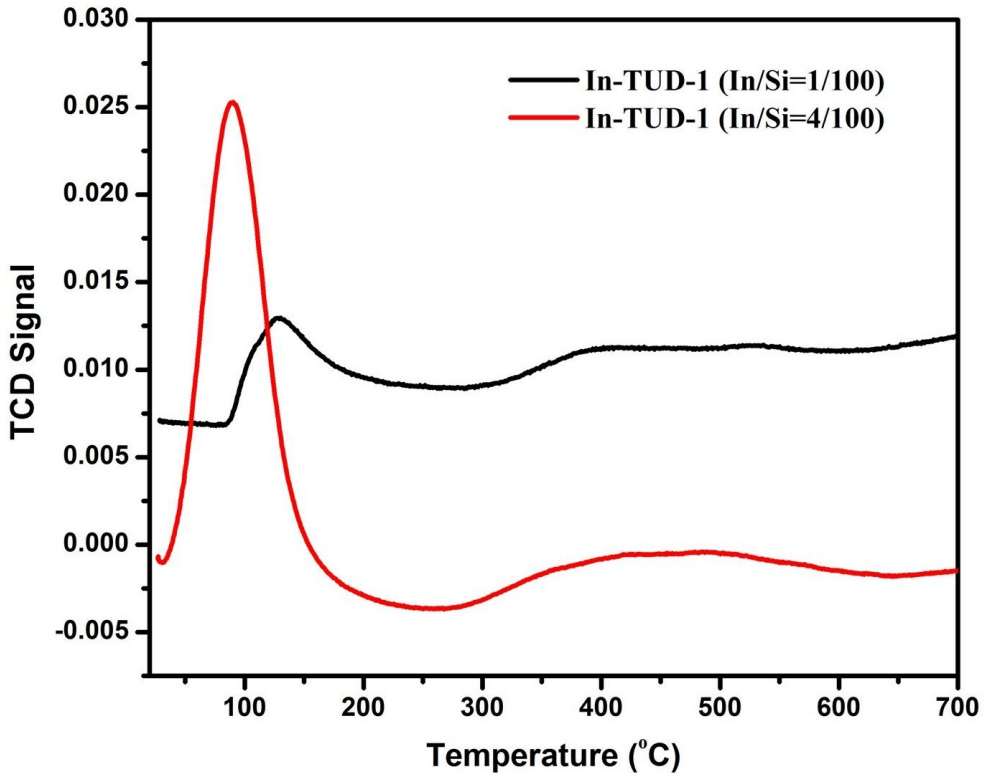

Fig. S6. Ammonia Temperature Programmed Desorption (TPD) profile.

Table S7. Order and rate constant determination.

Order(n)	A	Rate constant(k)	R^2
0	$(N_{styrene0} - N_{styrene})$	0.162	0.938
1	$\ln(\frac{N_{styrene0}}{N_{styrene}})$	0.027	0.951
2	$(\frac{1}{N_{styrene}} - \frac{1}{N_{styrene0}})$	0.004	0.961

.

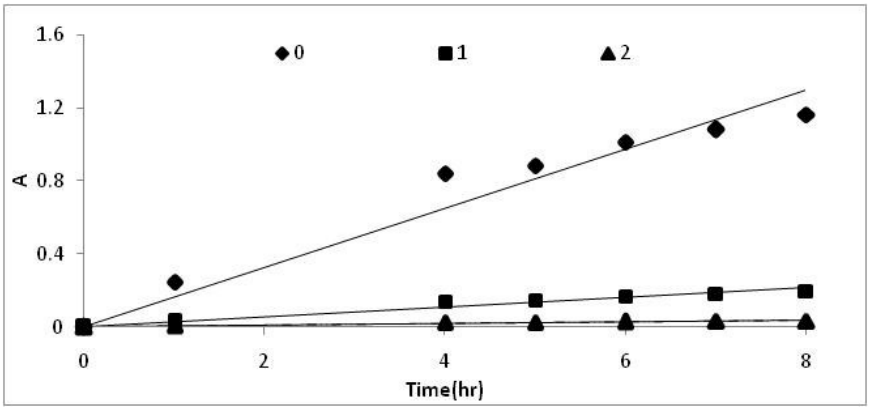

Fig. S8. Plot of A vs. Time (h) for styrene oxidation reaction in a batch reactor.

Table S9. Determination of lnk and 1/T for activation energy calculation.

T(K)	k(hr^{-1})	ln k	1/T
343.15	0.014	-4.2687	0.002914
363.15	0.019	-3.96332	0.002754
383.15	0.022	-3.81671	0.00261
403.15	0.027	-3.61192	0.00248
423.15	0.032	-3.44202	0.002363

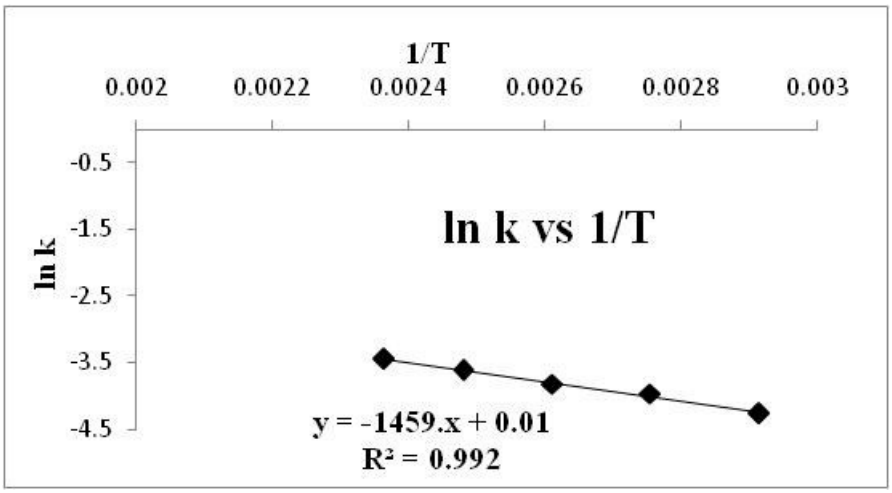

Fig. S10 Plot of lnk vs 1/T. The slope ($-E_a/R$) of quation of line is -1459. So, activation energy (E_a) of reaction is 12.13 kJ/mol.

Figure S11 The optimized structure for O_2 as adsorbate on SiO_2 surface with In_2O_3 nanoparticle along with partial charges on the atoms of adsorbed oxygen (using UFF method).