SUPPORTING INFORMATION

MnO_2 doped CeO_2 with tailored 3-D channel exhibit excellent performance for NH_3-SCR of NO

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MD Simulation

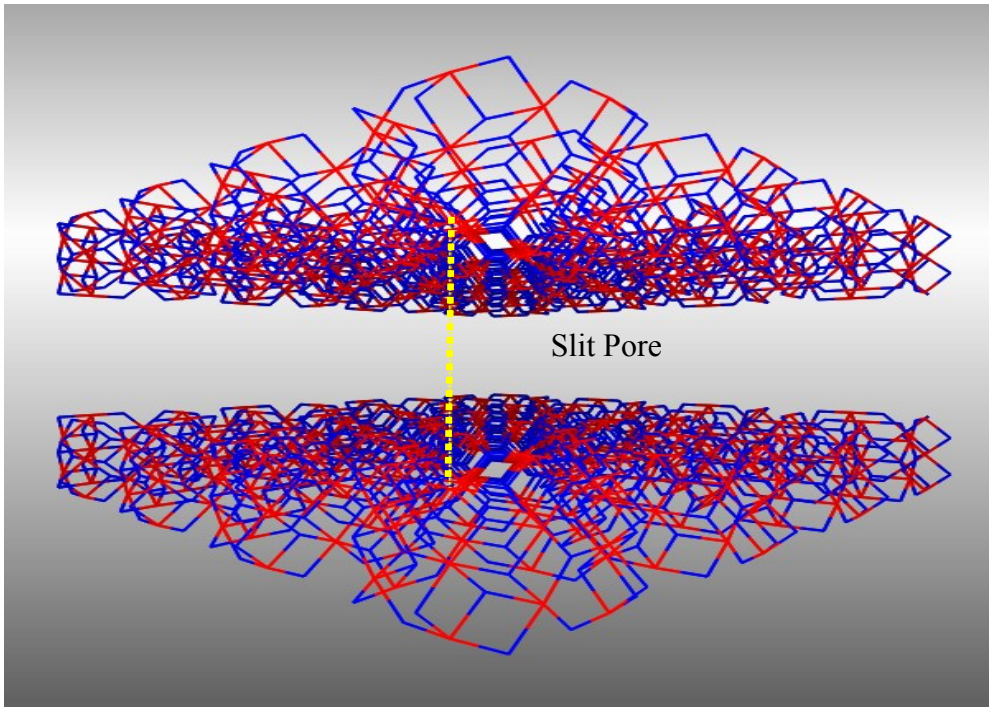
If the system is fluid, Mean square displacement (MSD) grows linearly with time. In this case it is useful to characterize the system behaviour in terms of the slope, which is the diffusion coefficient *D*

$$D = \lim_{t\to\infty} \frac{1}{6t} < |\mathrm{r(t)\text{-}r(0)}|^2 >$$

The average mean square displacement of all the atoms in a simulation can be easily computed by Monte Carlo method

The slit model were represented by two surface (0 0 1) of β MnO_2 with a gap (Scheme S1). The box consisted of 4 × 4 × 2 unit cells was used and periodic boundary conditions were applied in every direction for each simulation. Geometry optimization and charge allocation were calculated by Forcite and DMol3. Water molecule trajectories in the slits at 393 K under 0.06 bar were simulated by Forcite dynamics task. Universal Force Field was used for all the atoms and the Coulombic interactions were calculated using the Ewald summation method. A dynamic simulation runs using NVT Ensemble. Time-step is 0.1 fs and total simulation time is 15 ps.

Shown as Figure S1, at the beginning of 2ps, the plot of MSD is proportional to $t^{2,}$ which indicates that motion in this regime is not diffusive; it is in fact ballistic. The diffusion coefficient can be roughly estimate by calculating the slope of the linear portion of the curve.



Scheme S1. Slit pore model of MnO_2

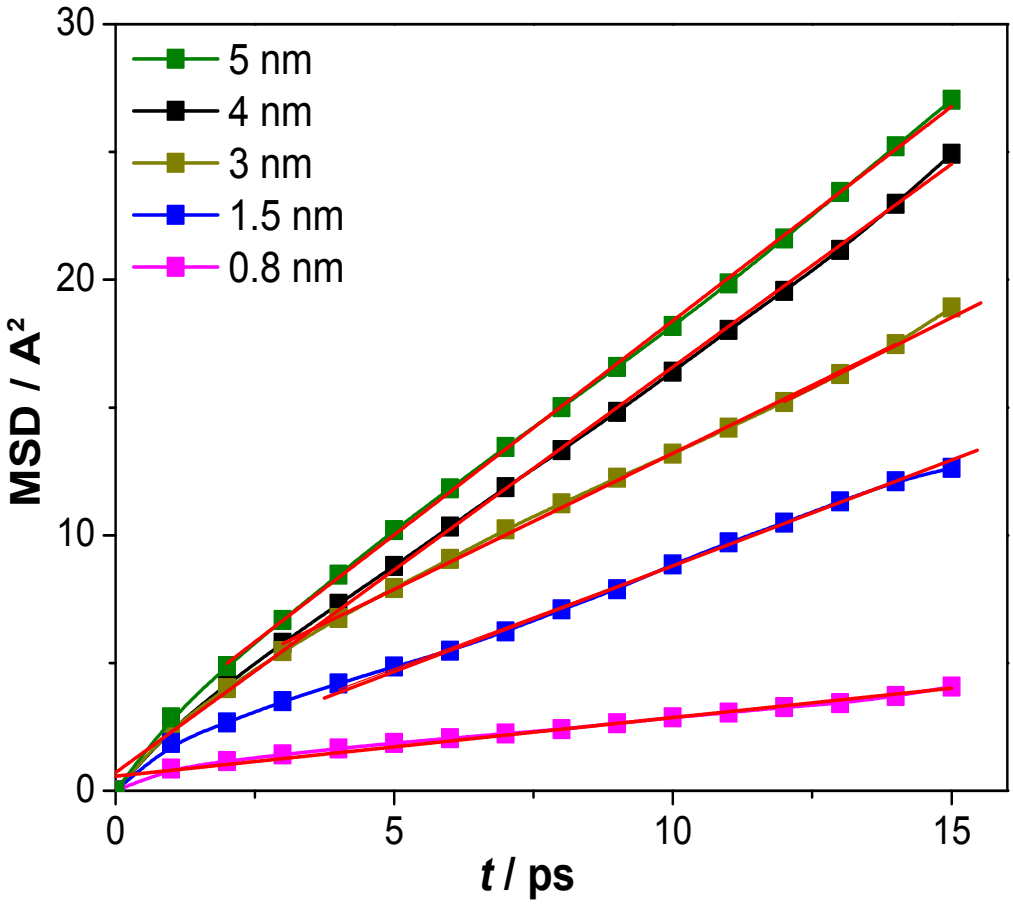


Figure S1 MSD curve of different model

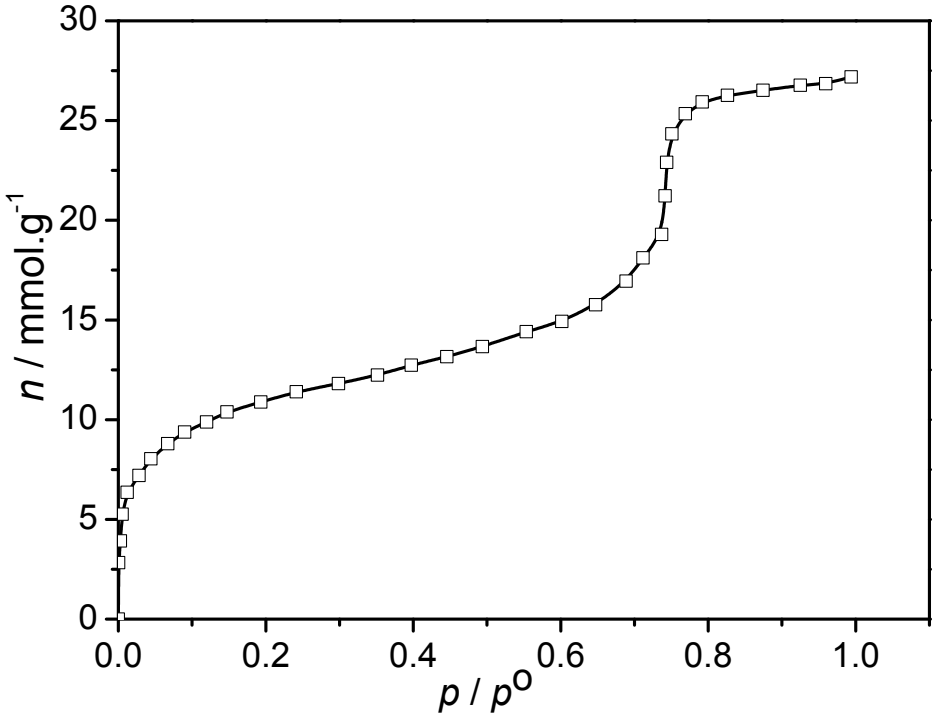


Figure S2 N_2 isotherm on KIT-6 at 77 K

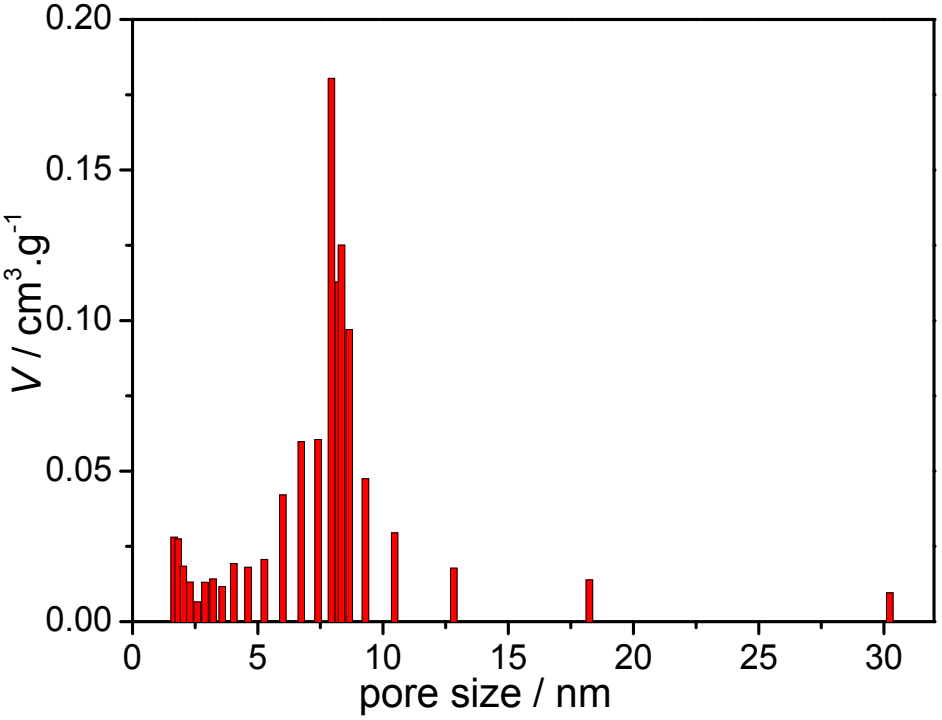
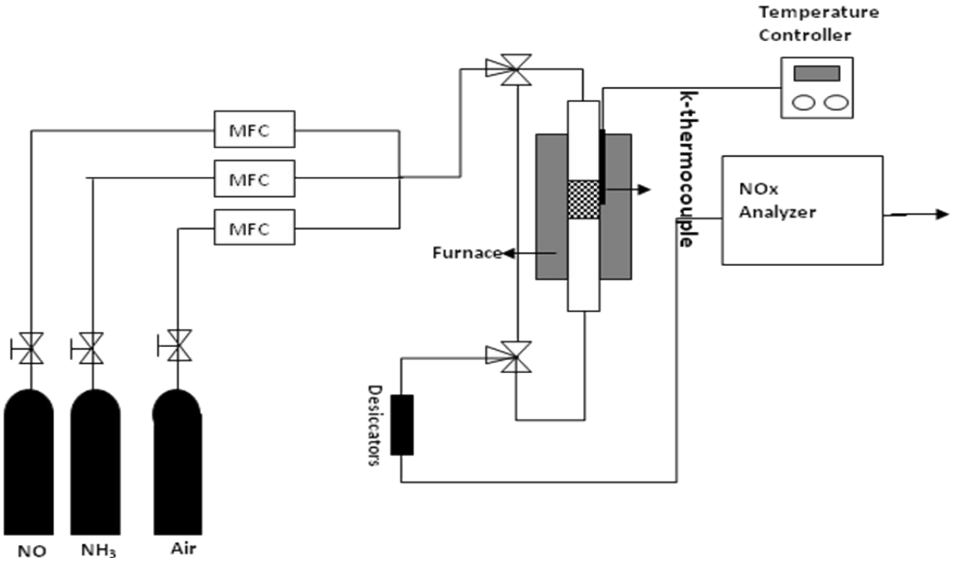


Figure S3. Porous distribution of KIT-6 calculated by BJH method



Scheme S2. The denitrification system of SCR

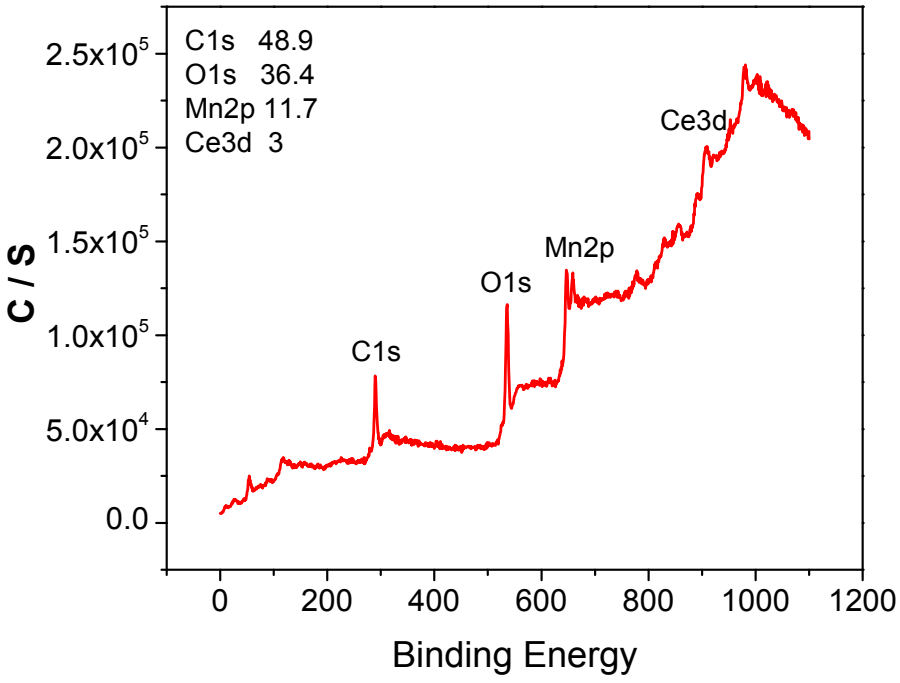


Figure S4. C1s O1s Mn2p Ce3d from XPS spectraof meso-porous MnO_2 doped CeO_2

Table S1. Water diffusion coefficients at 393 K under 0.006 bar (simulation results)

Slit size (nm)	0.8	1.5	3	4	5
Diffusion coefficient (10^{-5} cm^2s^{-1})	0.335	1.35	1.75	2.63	2.78

Table S2 Data for kinetic calculation

T,^{o}C	1/T ,K	η_{NO}	ln(-ln(1- η_{NO}))
75	0.0028736	0.05714	-2.83298
100	0.002681	0.25429	-1.22616
125	0.0025126	0.50875	-0.34136
150	0.0023641	0.72571	0.257405
175	0.0022321	0.85153	0.645727

Table S3 Results of kinetic calculation

Temperature range	Slop	intercept	Ea(kJ/mol)	P
T (125 ^{o}C-175 ^{o}C)	-3530.0	8.55	29.3	26.14
T (75 ^{o}C -125 ^{o}C)	-6936.3	17.18	57.7	146554.24