

Supplementary Information

Enhanced hydrogen separation performance of vertically-aligned carbon nanotube membrane with zeolite imidazolate frameworks surface modification

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Table S1. Detailed results of Rietveld refinement of ZIF-8

Site	Np	x	y	z	Atom	Occ	Beg
Zn	12	0.50000	0.00000	0.75000	Zn+2	1	4.531
N	48	0.41082	0.96641	0.68191	N	1	1.466
C1	24	0.37670	0.00560	0.62330	C	1	0.5365
C2	48	0.37010	0.89460	0.68710	C	1	3.987
C3	24	0.40500	0.08600	0.59500	C	1	-1.751
H1	48	0.38290	0.85310	0.72940	H	1	20
H2	48	0.56940	0.11960	0.36190	H	1	20
H3	24	0.55230	0.08070	0.44770	H	1	20

Phase name	Structure
R-Bragg	3.702
Spacegroup	I-43m
Scale	2.02151844e-006
Cell Mass	2731.009
Cell Volume (Å ³)	4929.11601
Wt% - Rietveld	100.000
Crystallite Size	
Cry size Lorentzian (nm)	93.6
Strain	
Strain L	0.00644345
Crystal Linear Absorption Coeff. (1/cm)	18.815
Crystal Density (g/cm ³)	0.920
Lattice parameters	
a (Å)	17.0185680

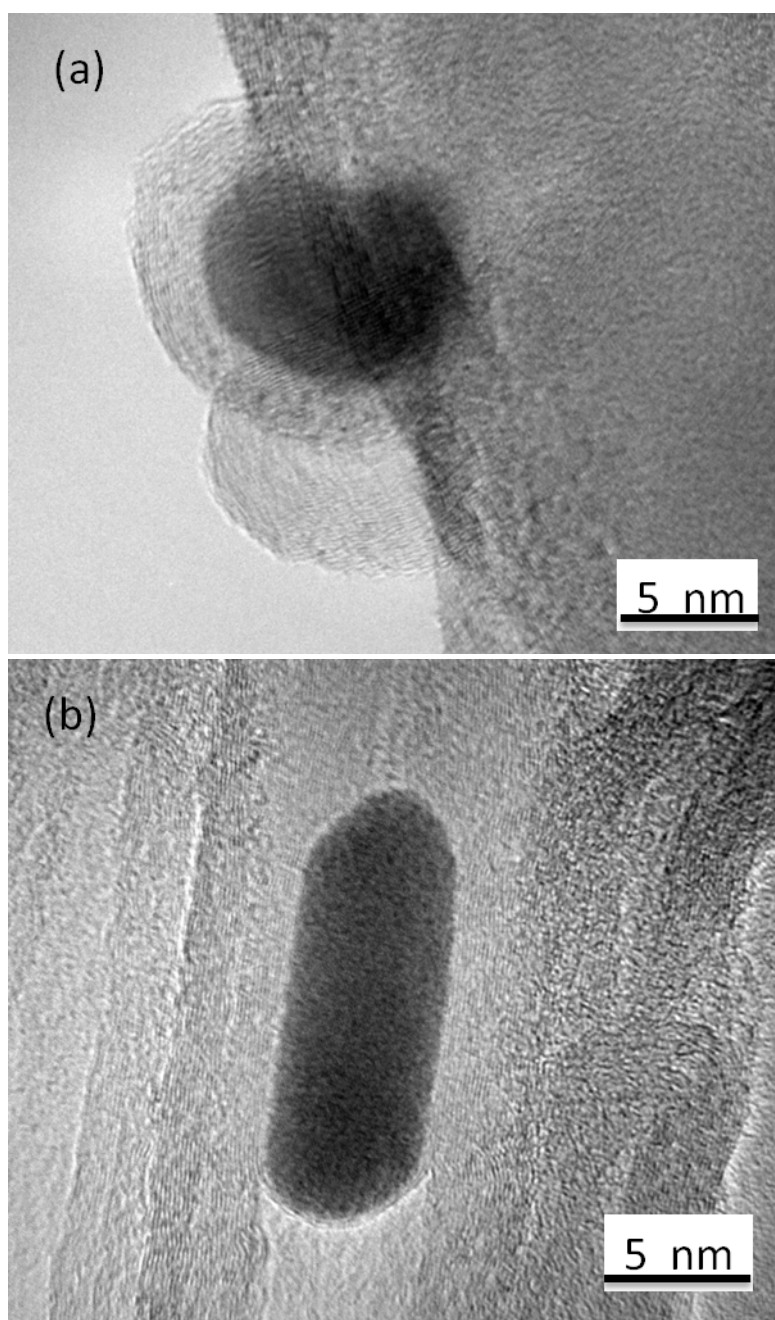


Fig.S1 (a) Typical HRTEM image for (a) iron catalyst on the surface of CNTs and (b) iron catalyst migrated into the channel