Electronic Supplementary Information

Direct Synthesis of Hydrothermally Stable Ge-IWR Zeolite

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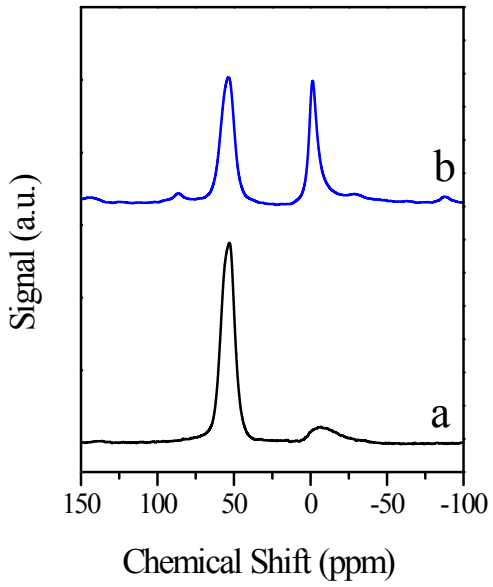

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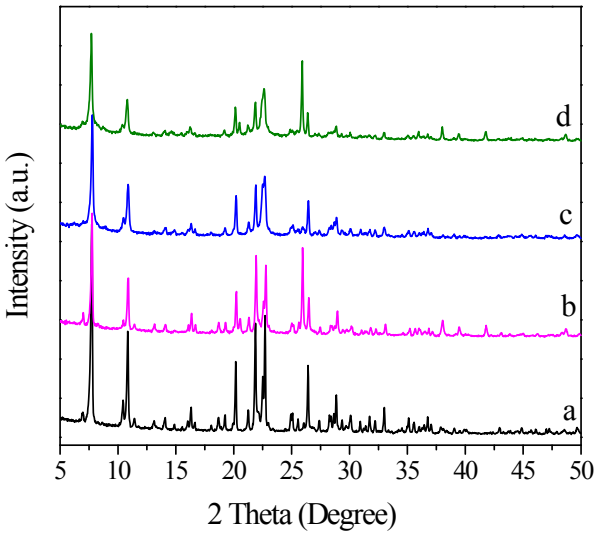
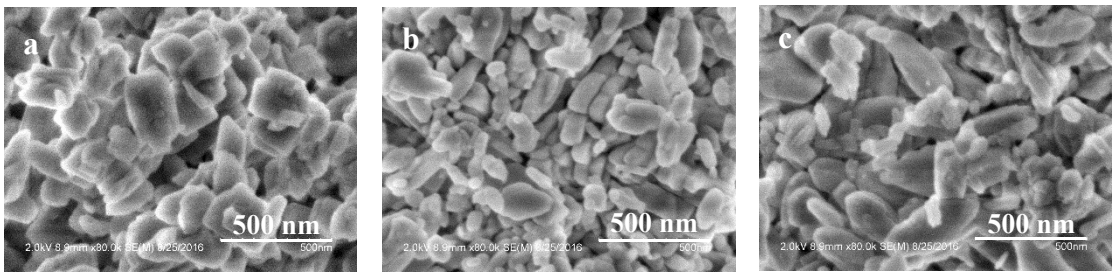
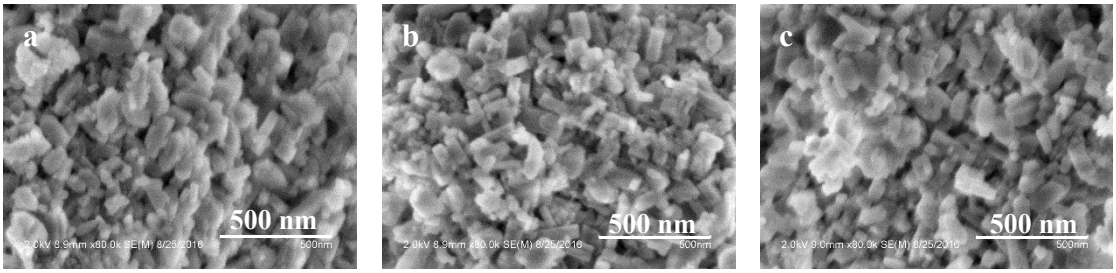


Fig. S2 XRD patterns of Al-free-IWR zeolite: calcined (a), HNO_3 treated (b) and Al-IWR-50 zeolite: calcined (c), HNO_3 treated (d).

Al-free-IWR



Al-IWR-50



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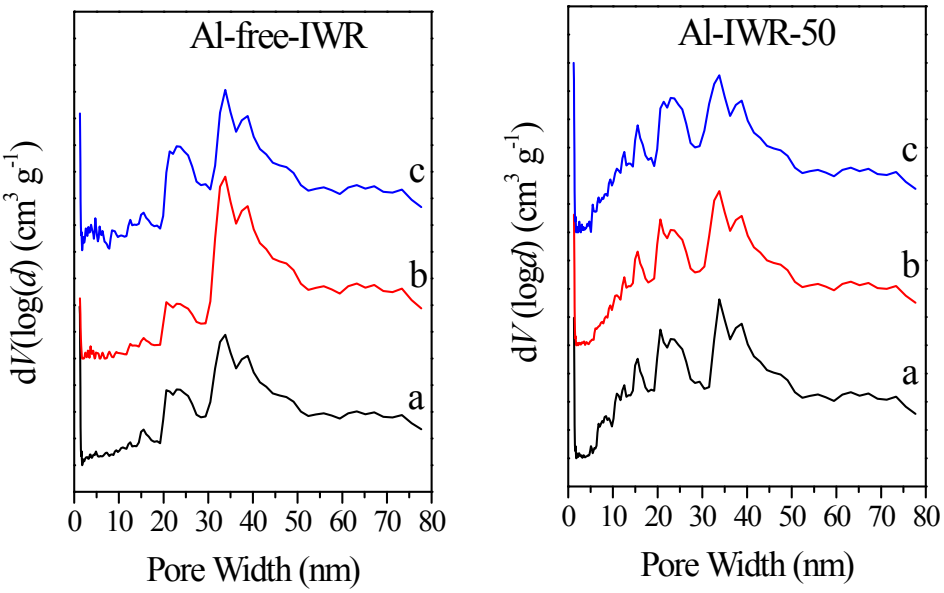

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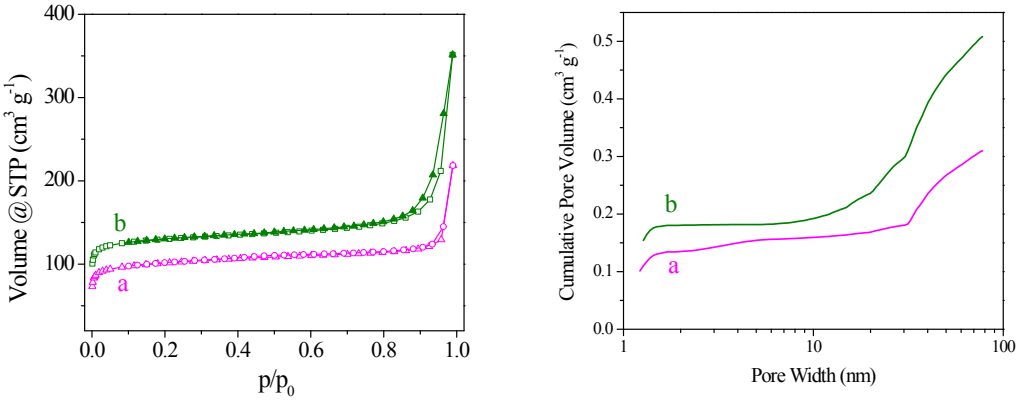

Fig. S5 N_2 adsorption-desorption isotherms (left) and NLDFT cumulative pore volume plots over the entire pore width range (right) of HNO_3 treated Al-free-IWR (a) and Al-IWR-50 (b).

Table S1 Survey of synthesis of IWR zeolites (423 K, 7 d)[a].

Si/Ge	H_2O/Si	SiO_2/Al_2O_3	Zeolite Phase
10	5.5	∞	AST
5	5.5	∞	CDO
2	5.5	∞	IWR + AST
10	5.5	250	IWR + CDO
5	5.5	250	IWR + CDO
2	5.5	250	IWR
2	5.5	100	IWR
2	5.5	50	IWR
2	5.5	25[b]	LEV
1	5.5	250	IWR
0.5	5.5	250	IWR
0.2	5.5	250	IWR
5	10	250	MFI
2	10	250	MFI
5	15	250	MFI
2	15	250	MFI

[a] The molar ratio of DEDMAOH/Si was fixed at 0.5.

[b] Isoproprate was used as aluminum source.

Table S2 Crystallographic data of Al-IWR-50.

Chemical composition: $H_{1.64}[Si_{41.86}Ge_{12.5}Al_{1.64}O_{112}]$

Refined composition: $Si_{42.57}Ge_{13.43}O_{112}$

Unit cell:

Space group *Cmmm* (No. 65)

a = 21.3126(4) Å

b = 13.5299(9) Å

c = 12.6615(2) Å

V = 3651.0(75) $Å^3$

Refined 2 θ range: 9-72

R_{wp} = 0.1079

R_p = 0.0854

Chi^2 = 3.122

Table S3 Atomic coordinates for Al-IWR-50 with e.s.d.'s in parentheses as obtained from Rietveld refinement.

Atom	Multiplicity	x/a	y/b	z/c	Occupancy
Si1	16*r*	0.07454(5)	0.1113(8)	0.3710(3)	0.436(1)
Ge1	16*r*	0.07454(5)	0.1113(8)	0.3710(3)	0.563(9)
Si2	16*r*	0.1487(8)	0.1987(9)	0.19129(1)	1.0
Si3	16*r*	0.2807(2)	0.1098(7)	0.1290(3)	0.968(9)
Ge3	16*r*	0.2807(2)	0.1098(7)	0.1290(3)	0.031(1)
Si4	8*p*	0.07282(5)	0.1211(4)	0	0.511(0)
Ge4	8*p*	0.07282(5)	0.1211(4)	0	0.489(0)
O1	16*r*	0.1057(8)	1.1708(6)	0.0950(11)	1.0
O2	4*i*	0	0.1238(2)	0	1.0
O3	4*g*	0.0885(20)	0	0	1.0
O4	8*q*	0.1032(3)	0.1108(3)	0.5	1.0
O5	8*o*	0.0763(83)	0	0.3382(4)	1.0
O6	16*r*	0.1236(4)	0.1878(2)	0.3050(6)	1.0
O7	8*n*	0	0.1421(6)	0.3349(4)	1.0
O8	16*r*	0.2224(2)	0.1252(6)	0.1757(5)	1.0
O9	16*r*	0.1676(7)	0.3115(6)	0.1723(8)	1.0
O10	8*o*	0.2965(1)	0	0.1656(3)	1.0
O11	8*p*	0.2710(2)	0.1276(2)	0	1.0

Table S4 Results of alkylation of benzene with ethylene over Al-IWR-50.

Time-on-stream (min)	Conversion (%)	Selectivity (%)	
		Ethylbenzene	Ethyl group
60	79.1	72.6	100
120	77.8	72.2	100
180	76.8	72.1	100
240	74.9	72.2	100
300	72.8	72.4	100
360	70.0	72.8	100
420	67.4	73.2	100
480	63.8	73.5	100

Reaction conditions: Temperature 473 K, pressure 3.5 MPa, WHSV 6 h^{-1}, Benzene/Ethylene 3.0.

Table S5 Textural properties of HNO_3 treated Al-free-IWR and Al-IWR-50.

Sample		Surface Area ($m^2\ g^{-1}$)		Pore Volume ($cm^3\ g^{-1}$)		
		S_{BET}[a]	$S_{m.}$[b]	$V_{t.}$[c]	$V_{m.}$[b]	$V_{m\text{-}NLDFT}$[d]
Al-free-IWR	HNO_3 treated	379	346	0.34	0.15	0.13
Al-IWR-50	HNO_3 treated	487	441	0.54	0.18	0.18

[a]BET surface area calculated from the N_2 adsorption data using the BET equation, [b]Micropore surface area and micropore volume estimated using the *t*-plot method, [c]Single-point total pore volume at P/P_0 = 0.99, [d]micropore volume calculated from NLDFT cumulative pore volume for pores below 2 nm in diameter.