Electronic Supplementary Material (ESI) for Environmental Science: Atmospheres.

Supporting information

Enhanced adsorption performance for aromatic sulfur compounds over hierarchical structure AgX zeolite

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Table S1. Textural properties of parent NaX zeolite and NaX-CA(3.0) adsorbent.

Adsorbents	Surface area (m^2/g)		Pore volume (cm^3/g)		Pore width (nm)		
	Micro-pores	Meso-pores	Micro-pores	Meso-pores	Micro-pores	Meso-pores	Average-pores
NaX	745.89	34.01	0.279	0.035	0.66	--	1.67
NaX-CA(3.0)	852.13	43.06	0.319	0.045	0.66	3.9	1.78

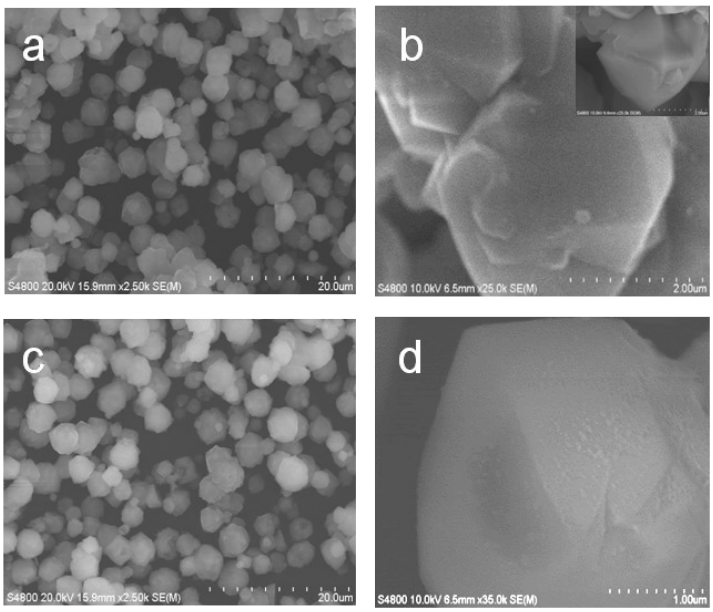

Fig. S1 SEM images of original NaX (a, b) and NaX-CA(3.0) zeolite (c, d) adsorbents.

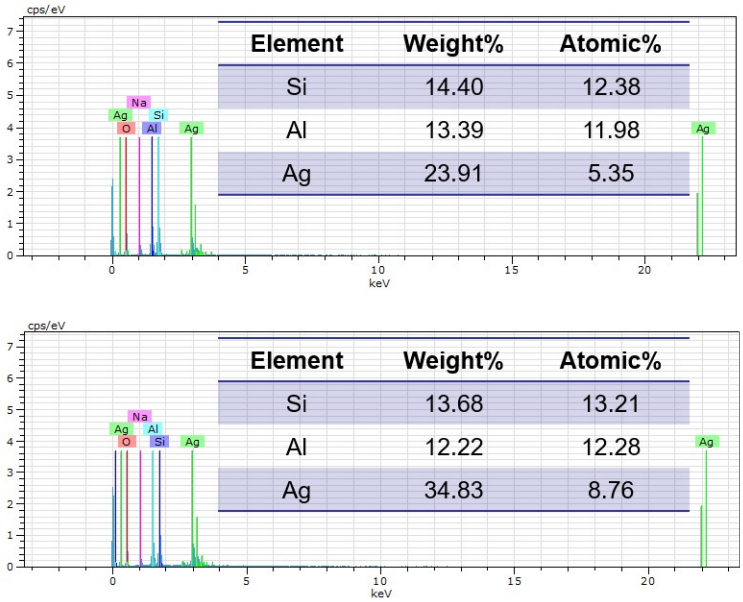

Fig. S2 EDS analysis of AgX and AgX-CA(3.0).

Table S2. H_2-TPR results of the adsorbents.

Sample	Temp.(℃)	Peak quantity(mmol/g)	The total peak quantity(mmol/g)
AgX	120	3.08	13.07
	221	2.16	
	309	2.48	
	412	5.35	
AgX-CA(1.5)	123	2.78	12.52
	225	2.12	
	295	2.67	
	407	4.95	
AgX-CA(2.0)	109	2.67	13.21
	224	2.25	
	303	3.18	
	405	5.11	
AgX-CA(3.0)	84	3.29	17.40
	200	1.91	
	279	3.43	
	400	8.77	

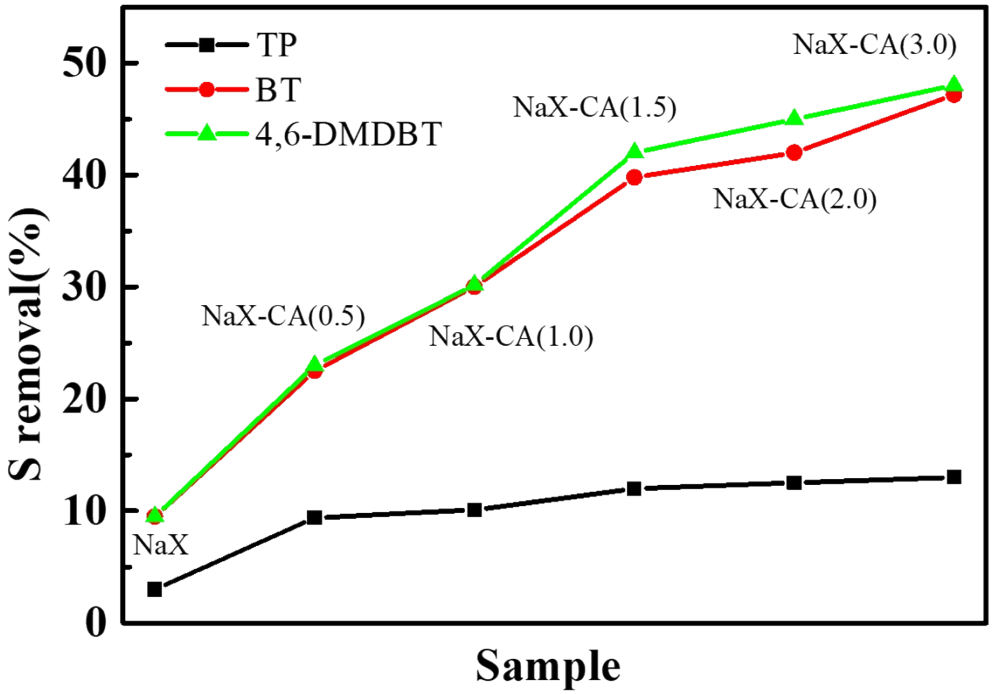

Fig. S3 The sulfur removal over NaX and NaX-CA(M) from model gasoline. Experimental conditions：Initial sulfur concentration was 20 ppm, Vol. (model gasoline) = 10 mL, W_t. (adsorbent) = 0.1 g, temperature: 80°C, contact time: 2 h.

Table S3. Adsorption kinetic parameters obtained at different temperatures by non-linear fitting.

	Pseudo-first-order Model				Pseudo-second-order Model		
Temp.(°C)	q_e *exp(mg/g)*	$K_1(min^{-1})$	q_e *cal(mg/g)*	R^2	K_2*(g/g min)*	q_e *cal(mg/g)*	R^2
80	1.941	0.245	1.959	0.898	0.204	1.967	0.998
50	1.456	0.126	1.256	0.892	0.157	1.513	0.997
30	0.131	0.114	0.104	0.878	0.054	0.125	0.990

Table S4. Langmuir and Freundlich isotherm parameters for sulfur compounds adsorption on AgX-CA(3.0) adsorbent.

	Langmuir Model			Freundlich Model		
Simple	K_L	q_m, (mg g^{-1})	R^2	n	K_F	R^2
BT	9.39	2.32	1	1.83	2.06	0.701
4,6-DMDBT	2.34	4.81	0.993	5.39	3.12	0.727

Table S**5**. The comparison of adsorption desulfurization performance of AgX-CA(3.0) with some representative Zeolite-based absorbents.

Adsorbents	Sulfur concentration (PPM S)	Model solvent/aromatics	Sulfur removal (%)	Capacity (mg S per g)	Breakthrough ($mL\ g^{-1}$)	Ref
AgX-CA(3.0)	10(BT)	n-Heptane	85.5	—	—	This work
AgX-CA(3.0)	10(DMDBT)	n-Heptane	99.1	—	—	This work
CeY	50(TP)	n-Octane	—	—	14.0	[1]
CeY	5(TP)	n-Heptane	80.0	1.2	—	[2]
Meso-Y	100(DBT)	n-Octane	—	—	17.0	[3]
Meso-CuCeY	100(DBT)	n-Octane	—	—	45.0	[3]
NaY	100(TP)	Cyclohexane	69.0	1.3	—	[4]
CeY	128(TP)	Cyclohexane	97.1	1.9	—	[4]
NaY	217(TP)	Benzene	—	0.1	—	[5]
HY	217(TP)	Benzene	—	0.1	—	[5]
NiY	217(TP)	Cyclohexane	—	3.1	—	[6]
CeY	217(TP)	Cyclohexane	—	2.4	—	[6]
CuCeY	142(TP)	n-Octane	—	—	36.0	[7]
CuCeY	142(BT)	n-Octane	—	—	195.0	[7]
Cu(II) CeY	142(TP)	n-Octane	—	—	20.0	[8]
AgY	142(TP)	n-Octane	—	—	75.0	[9]
AgCeY	142(TP)	n-Octane	—	—	25.0	[9]
CeY	142(TP)	Cyclohexane	—	2.3	—	[10]
AgCeY (Si/Al = 4.8)	142(TP)	n-Octane	—	—	30.0	[11]
CuBTC	250(BT)	n-octane	—	—	50.0	[12]
CuBTC	250(DBT)	n-octane	—	—	45.0	[12]
Cu_2O@HP-CuBTC	250(BT)	n-octane	—	—	65.0	[12]
Cu_2O@HP-	250(DBT)	n-octane	—	—	70.0	[12]

CuBTC						
Meso-ZnO/TiO2–SiO2	200(DBT)	n-octane	97.1	—	—	[13]
CN-x	200(DBT)	toluene	—	37.0	—	[14]

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