Supporting information

NaX zeolite framework containing of magnetic $MgFe_2O_4$/CdO nanoparticles: synthesis, characterization and catalytic performance in the decontamination of 2-chloroethyl phenylsulfide (2-CEPS) as a model of sulfur mustard agent

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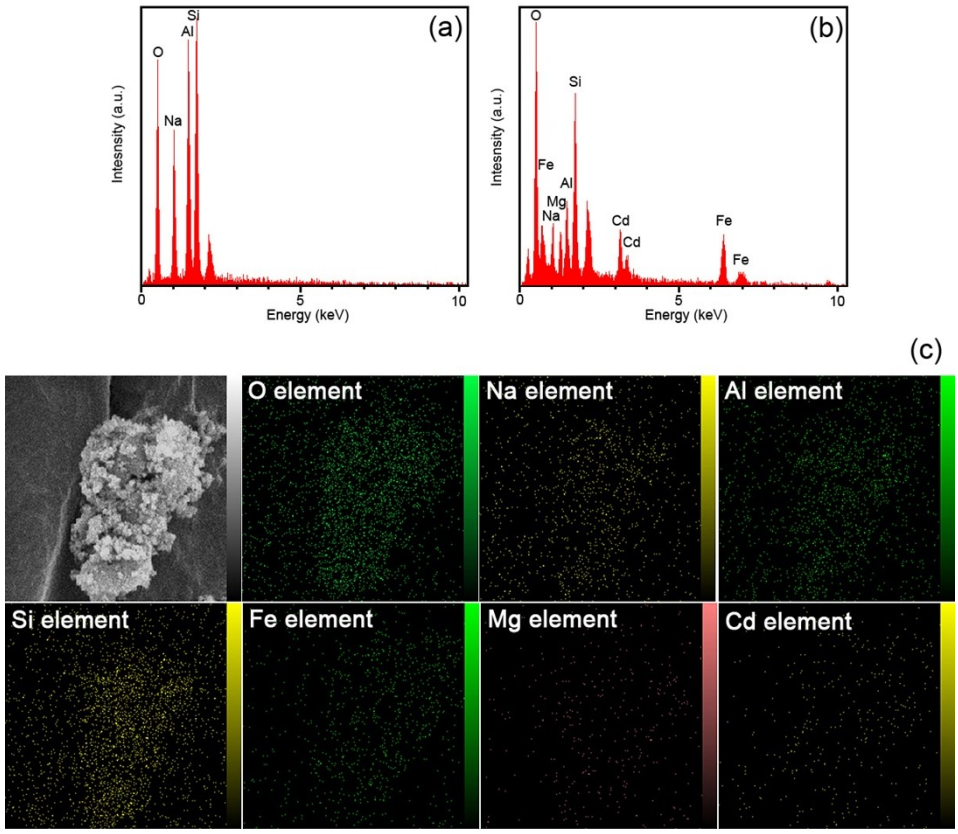

Fig. S1. EDAX analyses of: a) bare NaX and b) NaX/$MgFe_2O_4$/CdO. c) FESEM micrograph along with the EDAX elemental dot-mappings of the NaX/$MgFe_2O_4$/CdO.

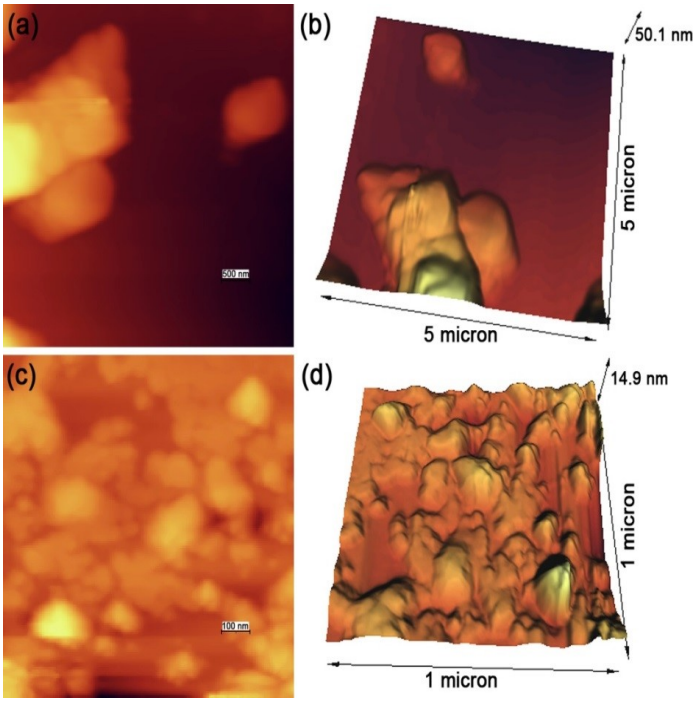

Fig. S2. 2D and 3D AFM micrographs of: a) and b) bare NaX, c) and d) NaX/$MgFe_2O_4$/CdO.

S1. GC-MS analysis

In order to precisely identify the 2-CEPS degradation products in the reaction with the zeolite NaX/$MgFe_2O_4$/CdO nanocomposite, a gas chromatography accompanied with mass spectrometry (GC-MS) analysis was utilized. As can be demonstrated in Fig.S3, the five specified peaks at different retention times were observed. The two peaks observed near 5.4 min and 8.3 min can be allocated to the n-heptane solvent and toluene internal standard, respectively. Furthermore, the three other characteristic peaks were recognized approximately 9.5 min to 12.2 min, which were corresponded to the 2-CEPS and its hydrolysis and elimination reaction products. Additionally, the mass spectra of 2-CEPS (m/z values 28, 45, 65, 109, 123, and 172) and its hydrolysis and elimination reaction products, involving 2-hydroxyl ethyl phenyl sulfide (2-HEPS) (m/z values 28, 43, 59, 85, 131, and 154) and phenyl vinyl sulfide (PVS) (m/z values 28, 39, 51, 65, 77, 91, 109, and 135) were clearly detected, respectively.

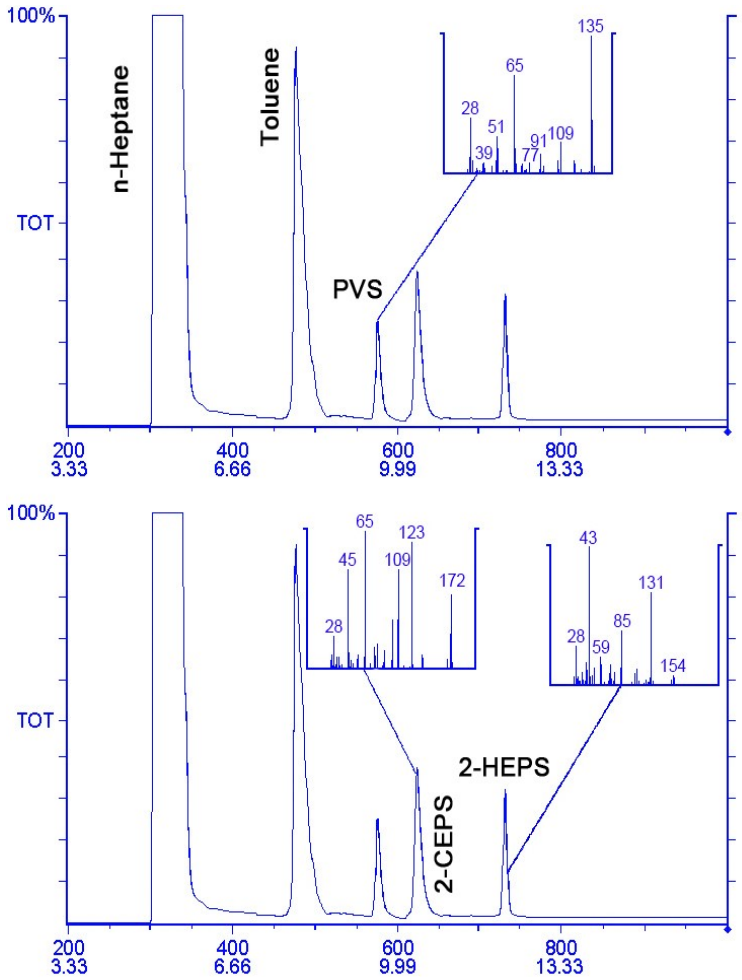

Fig. S3. GC-MS analysis and mass spectra of the 2-CEPS decontamination over the NaX/$MgFe_2O_4$/CdO.

Table S1. The EDAX analysis data for the NaX/$MgFe_2O_4$/CdO.

Element	Line	Atomic%	Weight%
O	Ka	75.72	60.40
Na	Ka	6.68	7.66
Al	Ka	4.03	5.42
Si	Ka	8.36	11.71
Fe	Ka	3.21	8.93
Mg	Ka	0.72	2.13
Cd	La	1.28	3.76
Total	-	100.00	100.00

Table S2. The acquired data from the N_2-BET, BJH and t plots corresponded to the as-synthesized catalysts at 77 K.

Sample	a_s, BET [$m^2\ g^{-1}$]	V_{me} [$cm^3(STP)g^{-1}$]	V_{mi} [$cm^3(STP)g^{-1}$]	Total pore volume [$cm^3\ g^{-1}$]	Average pore diameter [nm]
zeolite NaX	359.18	1.34	0.11	1.45	12.53
NaX/$MgFe_2O_4$/CdO	141.34	0.85	0.01	0.86	8.75

Table S3. GC-FID outcomes for the decontamination of 2-CEPS over the $NaX/MgFe_2O_4/CdO$ at different time intervals (optimal conditions; solvent: n-heptane, catalyst dosage: 50 mg).

Time Intervals (min)		2-CEPS (AUC_a)	Toluene Internal Standard (AUC_b)	Surface Ratios (AUC_a:AUC_b)
i	0	398623	349175	1.1416
ii	20	190275	274409	0.6934
iii	40	143172	258621	0.5536
iv	60	73390	232764	0.3153
v	80	53659	235700	0.2267
vi	100	46861	459875	0.1019
vii	120	00000	345772	0.0000

Table S4. First-order kinetic parameters for the decontamination of 2-CEPS in the presence of different catalysts (optimal conditions; reaction time: 120 min, solvent: n-heptane, catalyst dosage: 50 mg).

Catalyst type	Apparent rate constant (k_{app}, min^{-1})	Half-life ($t_{1/2}$, min)	First order kinetic equation ($\ln C_o/C_t = k_{app}t \pm b$)
Without catalyst (blank)	00	00	$\ln C_o/C_t = 00$
bare CdO	0.003	231.00	$\ln C_o/C_t = 0.003t-0.010$
bare $MgFe_2O_4$	0.005	138.60	$\ln C_o/C_t = 0.005t-0.042$
bare NaX	0.007	99.00	$\ln C_o/C_t = 0.007t+0.067$
$MgFe_2O_4/CdO$	0.010	69.30	$\ln C_o/C_t = 0.010t+0.026$
NaX/CdO	0.012	57.75	$\ln C_o/C_t = 0.012t+0.012$
$NaX/MgFe_2O_4$	0.149	46.20	$\ln C_o/C_t = 0.149t-0.073$
$NaX/MgFe_2O_4/CdO$	0.219	31.64	$\ln C_o/C_t = 0.219t-0.026$