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Supporting Information

Visible Light Enhanced Removal of Sulfur Mustard Gas Surrogate from a vapor phase on Novel Hydrous Ferric Oxide/Graphite Oxide Composites

by

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Table S1. Peak positions and intensities (in parenthesis) of the pK_a distribution.

Sample	pH	pK_a 6-7	pK_a 7-8	pK_a 8-9	pK_a 9-10	pK_a 10-11	All
FeO	6.67		7.20 (0.069)	8.64 (0.069)	10.00 (0.153)		0.291
FeO-GO	6.67	6.57 (0.159)	7.69 (0.094)	8.830 (0.126)		10.23 (0.362)	0.742
FeO-GOU	6.71	6.67 (0.166)		8.15 (0.068)	9.13 (0.092)	10.39 (0.325)	0.651

Details in the Scherrer equation.

The Scherrer was used to calculate the sizes of the crystallites:

$$\tau = \frac{K\lambda}{\beta cos\theta}$$

Where:

τ is the mean size of the crystallite, λ is the wavelenght of the X-Ray source (0.154 nm), K is the shape factor (0.9), β is the line broadening at the half maximum intensity of the peak, and θ is the Bragg angle.

The β values of the FeO, FeO-GO, and FeO-GOU samples are: 2.96, 4.07, and 2.40 respectively. The maximum of the peak is located at 35.5 2θ. The crystallite values are 2.9, 2.1 and 4.0 nm respectively.

Details of the energy band gap calculation:

The remission of the Kubelka-Munk function was calculated according the formula:

$$F(R_\infty) = \frac{(1 - R_\infty)^2}{2R_\infty} \quad (1)$$

Where:

$$R_\infty = \frac{R_{sample}}{R_{standard}} \quad (2)$$

R_{sample} and $R_{standard}$ are the reflectivity of the sample and standard respectively. A standard of MgO was employed as a reference material.

The band gap (*Eg*) is related to the linear absorption coefficient (α), by the Tauc relation.

$$\alpha h\nu = C_1(h\nu - Eg)^{1/2} \tag{3}$$

Where *hv* is the photon energy and C_1 is the proportionality constant. When the material scatters in a diffuse manner, the absorption coefficient becomes equal to 2α , therefore:

$$[F(R_\infty)h\nu]^2 = C_2(h\nu - Eg) \tag{4}$$

The extrapolation of the linear fit of the plot of $[F(R_\infty)h\nu]^2$ versus the photon energy (*hv*) yields the value of the *Eg*.

Image processing of Figure 3

The selected section of the image was selected, the Fourier transform was transformed, and a band pass filter was applied in the Fourier transform. The inverse Fourier yield the image presented in Figure 3 (Figure S1).

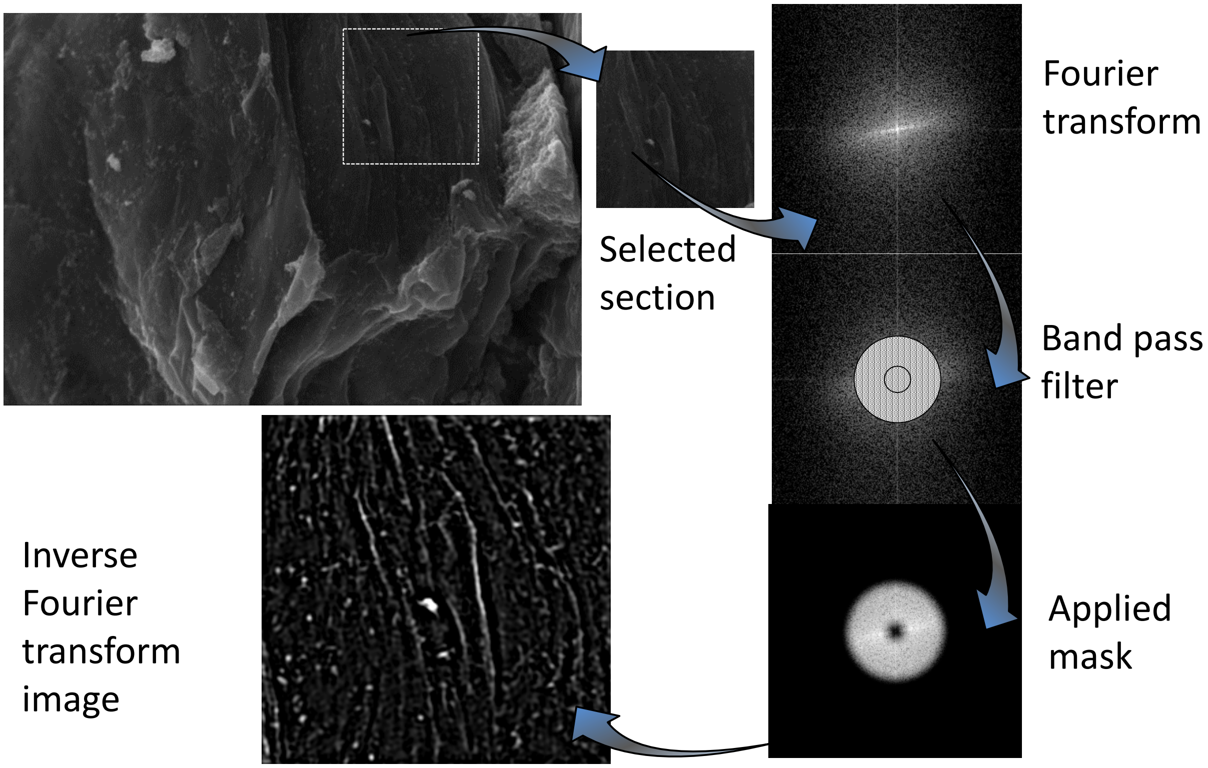

Figure S1. Image processing applied in Figure 3.

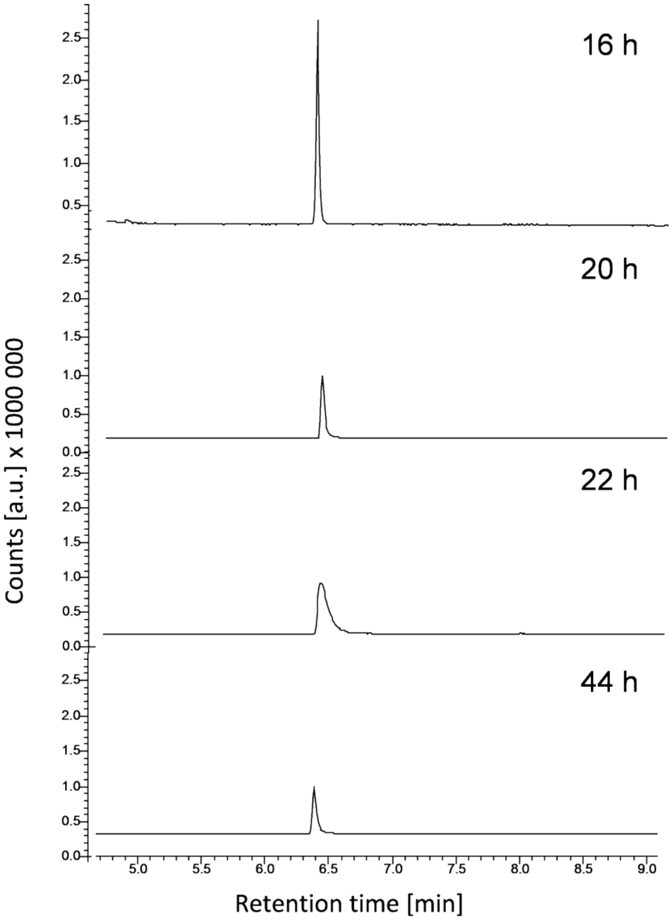

Figure S2. CEES chromatograms representing the concentration of CEES in the headspace of the reactors after 16, 20, 22 and 44 h of exposure. The intensity of the peak decreased with an increase in the reaction time, reaching a constant value after about 22 h. Since an increase in time up to 44 h did not significantly change the CEES concentration, 24 hours was accepted as a sufficient time to reach total CEES evaporation which lead to a constant concentration in our systems.