Electronic Supplementary Information for

Transformation of Mackinawite to Greigite by Trichloroethylene and Tetrachloroethylene

Ying Lan[1,2], Andrew S. Elwood Madden[3], and Elizabeth C. Butler[1,*]

Environmental Science: Processes and Impacts

* Corresponding author phone: +1 405 325 3606; Fax: +1 405 325 4217; email:

ecbutler@ou.edu

[1] School of Civil Engineering and Environmental Science, University of Oklahoma, Norman, Oklahoma, 73019, USA.
[2] Present address: Institute of Environmental Health, Oregon Health & Science University, Portland, Oregon, 97239, USA.
[3] School of Geology and Geophysics, University of Oklahoma, Norman, Oklahoma 73019, USA.

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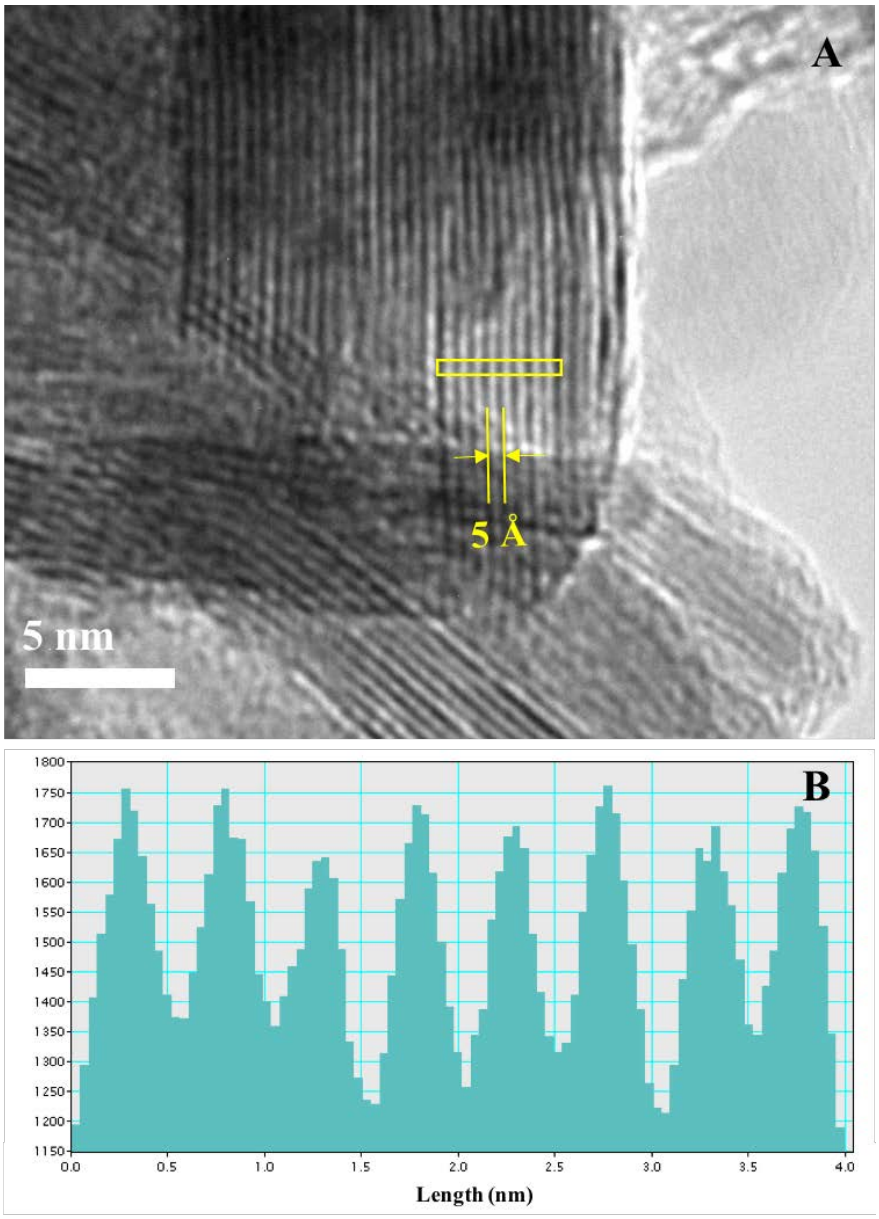


Figure ESI 1. Calculation of d-spacing using HRTEM images obtained from the FeS sample that reacted with PCE: (A) HRTEM image of FeS after reaction with PCE for seven weeks; (B) intensity profile from the atomic layers shown inside the yellow box in (A). The valleys in (B) correspond with the atomic layers shown in (A), and each peak represents one d-spacing between two atomic layers. The length of eight peaks equals 4 nm, so each peak is 5 Å long.

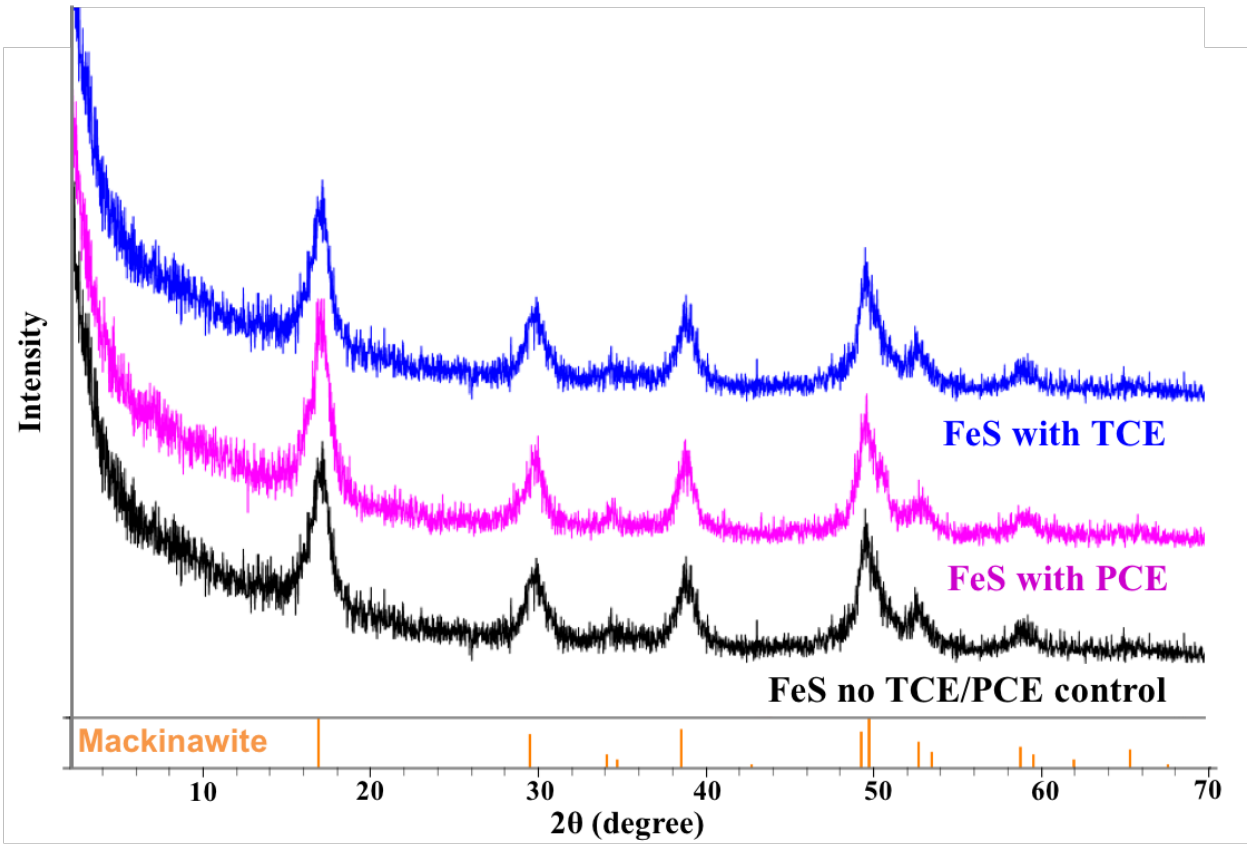
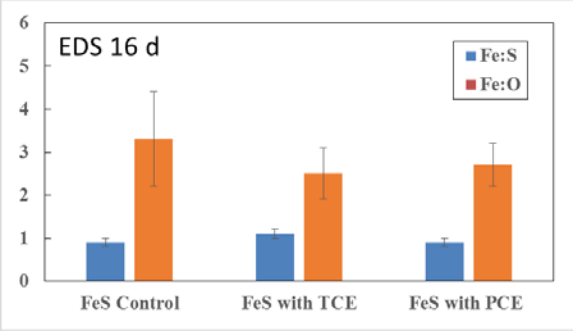
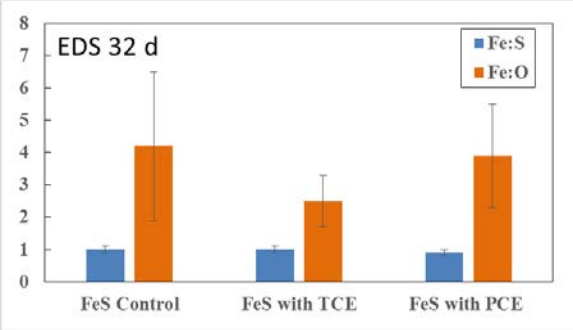


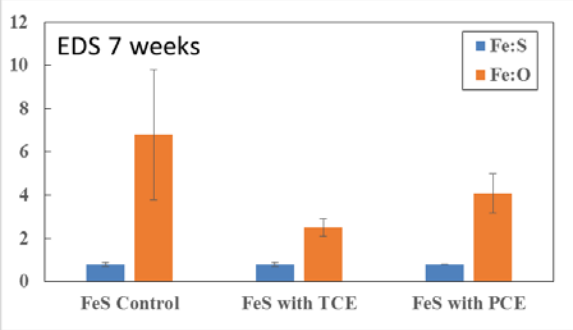
Figure ESI 2. XRD patterns of the FeS samples with TCE or PCE and the no TCE/PCE control at seven weeks.

Bulk FeS composition before and after reaction with TCE or PCE. EDS data were collected from randomly selected particles in all samples after 16 days, 32 days, and seven weeks. Particle sizes ranged from 20 to 150 nm and were selected randomly. The atomic percent of O, Fe, and S from EDS analyses were summed, normalized to 100%, and the ratios of Fe to O (Fe:O) and Fe to S (Fe:S) compared (Figure ESI 3). Other elements detected by EDS included C and Si. The source of Si was most likely Si-containing pump oil in the high vacuum systems of the HRTEM and SEM,[4] and the source of C was the Plexiglas chip and carbon tape (for SEM analysis) and holey carbon grids (for TEM analysis). There was no difference in Fe:S determined by EDS between the samples that reacted with TCE or PCE and the no TCE/PCE controls, and any trend in Fe:O among the samples was not statistically significant (Figure ESI 3).

[4] A. Kumao, H. Hashimoto and K. Shiraishi, *J Electron Microsc*, 1981, **30**, 161-170.







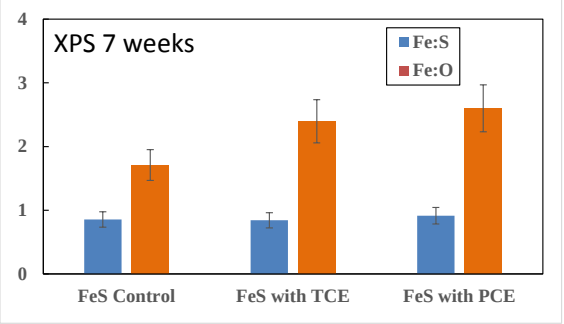


Figure ESI 3. Fe:S and Fe:O determined by EDS (top three panels) and XPS (bottom panel). Error bars in the top three panels represent the standard deviation of multiple (n) measurements (EDS 16 d, n=5-7; EDS 32 d, n=5-6; EDS 7 weeks, n=12-16). Error bars in the XPS results were calculated using propagation of error, assuming the standard deviation of the XPS results is 10%.

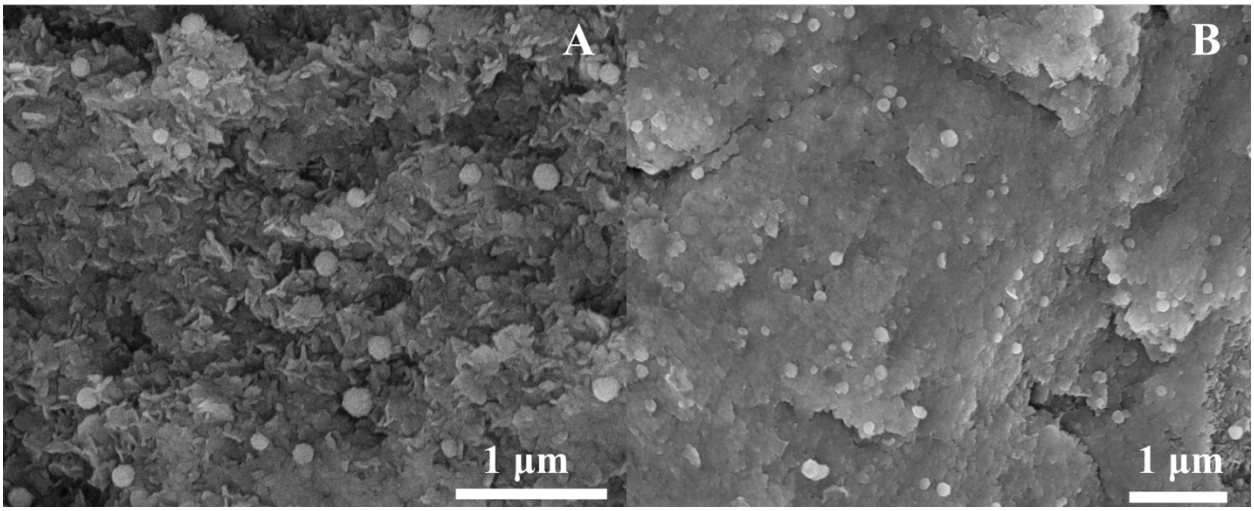


Figure ESI 4. SEM images of the surface of FeS after reacting with TCE for 32 d (A), and after reacting with PCE for 16 days (B).

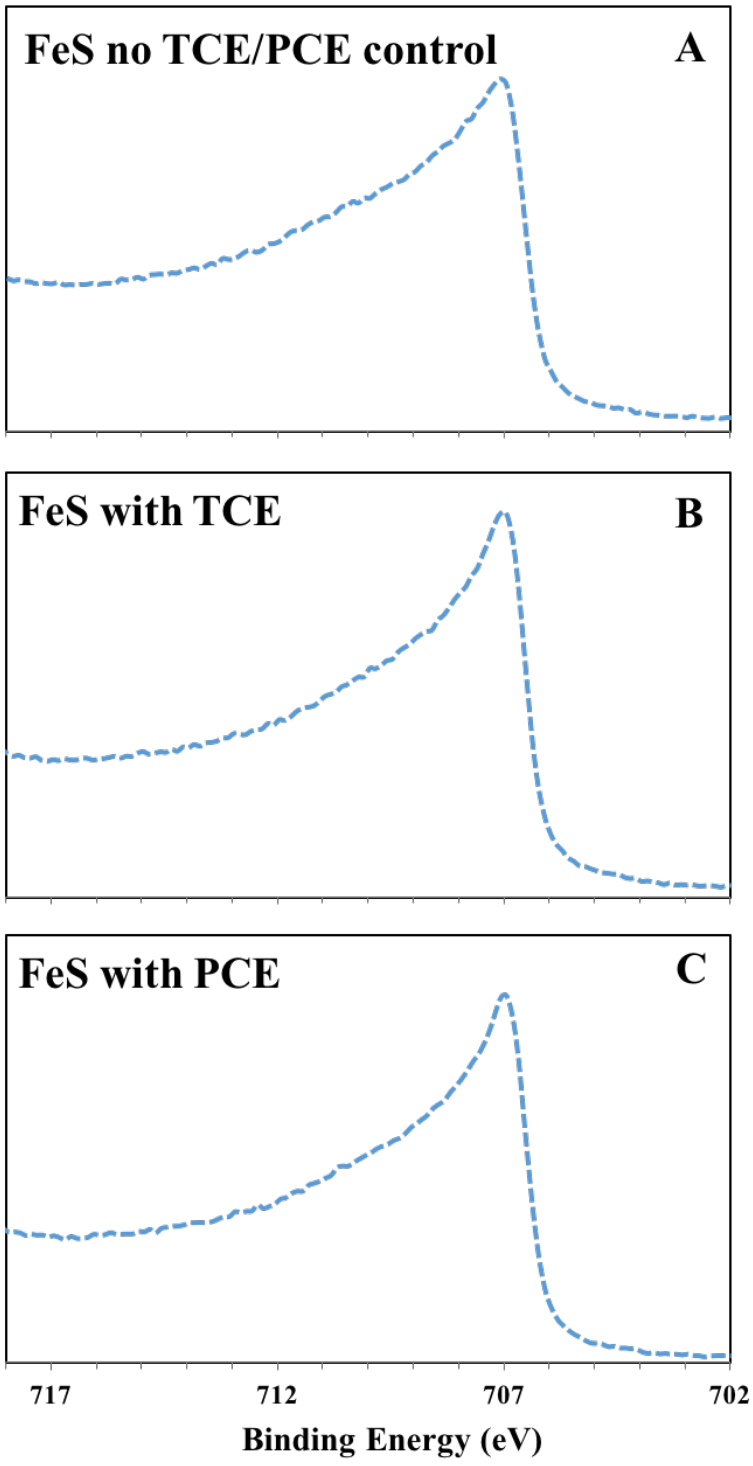


Figure ESI 5. The Fe $2p_{3/2}$ XPS spectra of FeS surface after seven weeks. (A) FeS no TCE/PCE control; (B) FeS with TCE; (C) FeS with PCE.