☒ **Talk** ☐ **Poster**

Identifying Redox Reaction Zones in Shale Using Multi-Energy Micro-XRF and XANES Linear Combination Fitting

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This presentation introduces a synchrotron-based analytical method that combines multi-energy micro-X-ray fluorescence (μ-XRF) mapping with linear combination fitting against reference XANES spectra to identify redox reaction zones in complex porous media. This approach enables spatially resolved, semi-quantitative speciation of redox-sensitive elements—for example, iron and sulfur—by collecting elemental maps at carefully selected incident energies near absorption edges. Unlike traditional EDS mapping, which provides elemental but not oxidation state information, this method distinguishes Fe(II)/Fe(III), or S(-II/IV) distributions at micrometer scales without requiring full XANES mapping. The technique has been successfully applied in several studies on shale–fluid interactions [1-5], revealing redox fronts, gradients, and mineralogical transformations in heterogeneous matrices. We further compare μ-XRF-derived maps with EDS to highlight the advantages and limitations of each method in interpreting reaction zones. While demonstrated in shale systems, this framework is broadly applicable to other environmental and engineered materials where redox dynamics control geochemical behavior.

References

[1] Li, Q., Jew, A. D., Kohli, A., Maher, K., Brown Jr, G. E., and Bargar, J. R. (2019). Thicknesses of chemically altered zones in shale matrices resulting from interactions with hydraulic fracturing fluid. Energy & Fuels, 33(8), 6878-6889.

[2] Xiong, W., Deng, H., Stuckman, M., Lopano, C., and Hakala, J. A. (2022). Fe oxidation and species distribution at the rock–fluid interface of marcellus shale reacted with hydraulic fracturing fluid. Energy & Fuels, 36(15), 8150-8160.

[3] Xu, Y., Arya, L., Rooney, C., Sharma, A., Liu, X., Hu, Z., Duan, X., Trelewicz, J.R. and Li, Q. (2024). Influence of fracturing fluids on shale matrix permeability and micro-mechanical properties after chemical interactions. Geoenergy Science and Engineering, 241, 213197.

[4] Li, Q., Jew, A.D., Kiss, A.M., Kohli, A., Alalli, A., Kovscek, A.R., Zoback, M.D., Cercone, D., Maher, K., Brown Jr, G.E. and Bargar, J.R. (2018, September). Imaging pyrite oxidation and barite precipitation in gas and oil shales. In Unconventional Resources Technology Conference, Houston, Texas, 23-25 July 2018.

[5] Jew, A. D., and Brownlow, J. W. (2025). Inorganic Alterations in Unconventional Shale Reservoirs: Importance of Additive and Base Fluid Chemistry. *Energy & Fuels*, *39*(8), 3799-3819.