

Emergent Properties in a Mixed Aqueous Mineral Sulfide System: An Opportunity to Accelerate Oxidative Decomposition of Persistent Organic Pollutants

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Since the discovery that pyrite, FeS_2 , produces hydrogen peroxide (H_2O_2) and hydroxyl radical (OH^*) when reacting with dissolved oxygen ($\text{O}_2(\text{aq})$) [1], there has been a flurry of research in which pyrite is explored as a reactant in the decomposition of pollutants. Pyrite reacts with $\text{O}_2(\text{aq})$ to form H_2O_2 , which reacts to form OH^* via the Fenton reaction [2]. OH^* is extremely reactive toward organic molecules and pyrite slurries have been demonstrated to decompose a wide range of organic pollutants. The widespread availability of fine-grained pyrite in coal and mine tailings makes it possible to use pyrite-driven OH^* formation at scale.

The $\text{O}_2(\text{aq})$ to H_2O_2 reaction is the slow step in the formation of OH^* in pyrite slurries. A subsequent study showed that combining pyrite with chalcopyrite, CuFeS_2 , leads to an unpredicted increase in the rate of hydroxyl radical formation [3], constituting an emergent property. The emergent property arises as the H_2O_2 formation is faster on the chalcopyrite surface than on the pyrite surface, but the conversion of H_2O_2 to OH^* is faster in the presence of pyrite than chalcopyrite alone.

More recently we have been able to use this emergent property in the pyrite-chalcopyrite system to accelerate the degradation of trichloroethene (TCE), a persistent organic pollutant found in the environment [4]. TCE is enhanced by pyrite-chalcopyrite mixtures, with 50-50 and 75-25 mixtures providing the highest degree of acceleration. The broader implication of this work is that redox systems involving multiple components and intermediate aqueous species can develop emergent properties. There is currently no framework to predict emergent properties in these types of systems.

The work on pyrite reactivity has its roots in earlier work at Penn State University under the direction of my PhD advisor Dr. Hubert L. Barnes.

References:

- [1] C.A. Cohn et al. *Geochemical Transactions* 7(2006).
- [2] Schoonen, M. A. et al. *GCA* **74**, 4971-4987.
- [3] Kaur, J. and M.A. Schoonen, *GCA* 2017. **206**: p. 364-378.
- [4] Kaur J. Mineral-Induced Reactive Oxygen Species (ROS) formation and its effect on Organic Pollutants and Human Health. (2016) Ph.D. Thesis, Department of Geosciences, Stony Brook University.