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Novel Metal Sulfides to Achieve Effective Capture and Durable Consolidation of Radionuclides

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Program: Separations and Waste Forms

ABSTRACT

This project evaluates chalcogels and other chalcogenide based materials as potential selective capture agents and as waste forms for iodine and for the capture of Cs, Sr and Co ions. The planned experiments focus on chemistries (for example Zn, Mo, W, Fe, Ni) and building blocks (for example $[\text{Sn}_2\text{S}_6]^{4-}$, $[\text{Mo}_2\text{W}_2\text{S}_6]^{4-}$, etc.) to create tailor-made chalcogels for selective capture of iodine and in order to determine the most effective material system. Also investigated are crystalline metal sulfide frameworks with ion-exchange properties designed specifically to capture Cs, Sr and Co radionuclide ions. We propose several approaches designed to produce functionalized materials tailored towards high selectivity for iodine and Cs, Sr and Co ions: 1) chalcogels with polarizable surfaces: physisorption of I_2 ; 2) oxidative coupling of terminal Q atoms in chalcogels to form Q-Q bonds (Q = S, Se); 3) reaction of I_2 with low oxidation state metals in chalcogels; and 4) crystalline metal sulfides as selective ion exchangers for Cs, Sr and Co removal; 5) conversion of the final products into glasses with the aim of developing systems with high chemical durability that can produce stable waste forms.

The proposed materials show great promise in capturing radionuclides even in dilute solutions and the project combines the considerable expertise of Northwestern University and PNNL in processing a variety of different chalcogel and chalcogenide materials, and ORNL's facilities to measure the sorption efficiency from simulated dissolver off-gas streams. Therefore, we bring a powerful meld of capabilities and synergies in this partnership. This broad, multifaceted project will help train students as the next generation of scientists versed in the materials science of the fuel cycle.