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Development of Novel Porous Sorbents for Extraction of Uranium from Seawater

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Collaborators: N/A

Program: MS: Fuel Resources

ABSTRACT:

As the uranium resource in terrestrial ores is limited, it is difficult to ensure long-term nuclear power generation. The oceans contain approximately 4.5 billion tons of uranium, which is one thousand times the amount of uranium in terrestrial ores, making the extraction of uranium from seawater a potentially attractive solution to developing sustainable nuclear fuel cycles. However, transformative technologies are needed in order to achieve economic uranium extraction. The objective of this proposed research is to develop highly porous sorbents for the extraction of uranium from seawater. We propose to accomplish this objective through design and investigation of new multifunctional uranyl chelators and engineering of nanoporous supports that facilitate cooperative sorbent interactions. Research performed during the last funding cycle using mesoporous materials and metal-organic frameworks (MOFs) provides a strong foundation for these studies as well as a baseline for sorbent performance. Density Functional Theory (DFT) calculations will be used to analyze ligands for uranyl binding strength, while promising organic functions can be readily grafted to mesoporous supports for performing sorption studies. A concerted effort will be directed at the development of rigid "lock and key" type pincer ligands, where organic functions are oriented to exploit kinetic and thermodynamic phenomena to effectively chelate uranyl. MOFs will be used as model platforms for probing cooperative binding interactions by multi-layer quantum mechanical/molecular mechanical (QM/MM) calculations, single-crystal X-ray diffraction, and X-ray absorption spectroscopy, to afford a detailed understanding of the molecular binding environment for uranyl. By judicious choice of ligand symmetry and metal, MOFs of varying topologies can be synthesized to elucidate the role of nanoporous supports in actinide extraction. Building upon the extremely promising sorption capacities demonstrated previously by MOFs and functionalized mesoporous carbon nanoparticles, additional research will focus on improving the grafting densities and stabilities for these materials to facilitate investigation under environmental conditions. Detailed uranyl sorption capacity, selectivity, and kinetics data will be obtained for all new materials. Promising candidates will be incorporated into nanocomposites for processing into stacks or braids for field tests in seawater and toxicity tests. This transformative research will significantly impact uranium extraction from seawater as well as benefit DOE's efforts on environmental remediation by developing new materials and providing knowledge for enriching and sequestering ultralow concentrations of other metals.