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Type: **Invited Lecture**

## INVITED LECTURE - Novel mesoporous materials for actinide and lanthanide separation

*Wednesday 19 September 2012 16:30 (20 minutes)*

We have undertaken the design, synthesis, and testing of reusable mesoporous materials for actinide and lanthanide separation, sequestration, and sensing. An experimental-computational collaboration has yielded several materials with a high binding capacity for  $^{239}\text{Pu}$ : functionalized mesoporous silica, mesoporous carbon, and ferrihydrite. Advances have been made with all three types of materials. The affinity for target actinides of several ligands grafted to mesoporous silica, as well as their binding geometry, has been predicted by ab initio relativistic density functional theory (DFT) geometry optimization calculations, and compared to experimental batch sorption and X-ray absorption spectroscopy (XAS) measurements. Additionally, these batch studies have established the ability to reuse the materials as high-capacity sorbents. Ordered mesoporous carbon (OMC) has proven far superior to activated carbon in terms of  $\text{Pu(VI)}$  capacity and sorption kinetics. Batch and XAS studies of mesoporous and nanoparticulate ferrihydrite interactions with  $\text{Pu(VI)}$  have revealed interesting light-induced redox chemistry at the iron-oxide surface that may yield separation capabilities. Alternative forms of these materials, such as monoliths and thin films, are being explored but functionalization is a major challenge. We are expanding our studies to different actinide and lanthanides ions and examine the effects of the presence of competing ions, as well as systematic ligand variation. We are exploring OMC-based electrodes offer a promising route for electrochemical separation and sensing of actinides and lanthanides.

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