Yucca Mountain Project

Radionuclide getter materials (collaboration with Sandia National Laboratory)

High temperatures and rad flux precludes the use of organic ligands

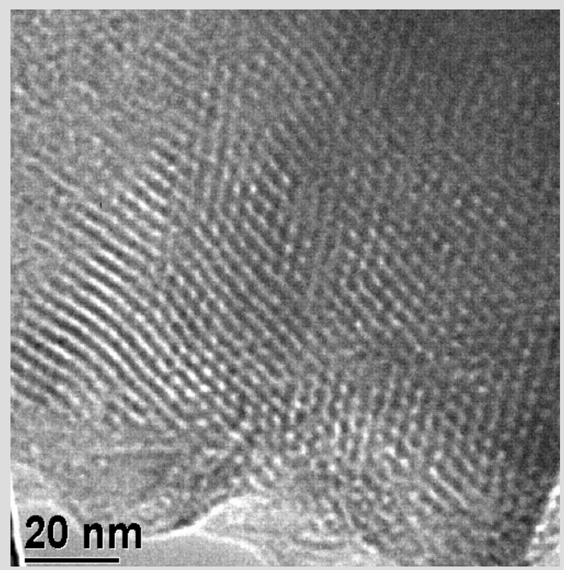
Yucca Mountain

Need nanoporous getter materials to sequester any radionuclides that might escape from the SNF in the repository

<u>Two parallel pathways:</u>

•Nanoporous ceramic oxides coated with reactive interfaces (SNL)

•Nanoporous metal phosphates (PNNL)

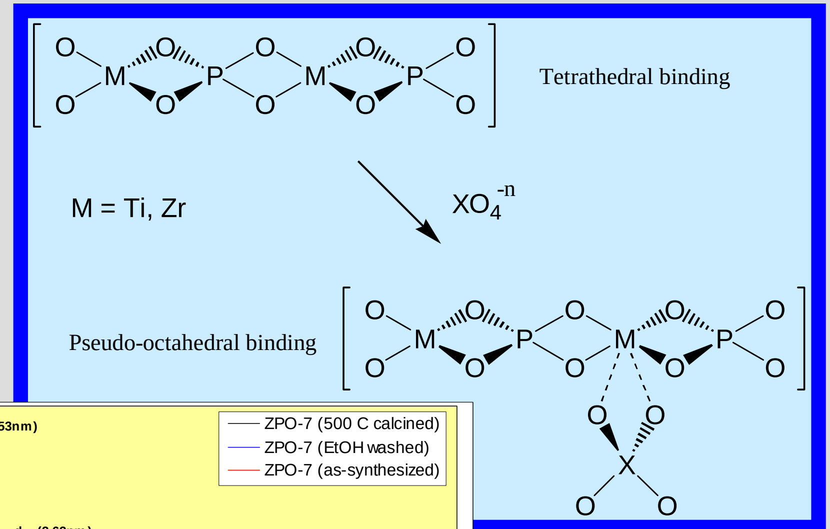


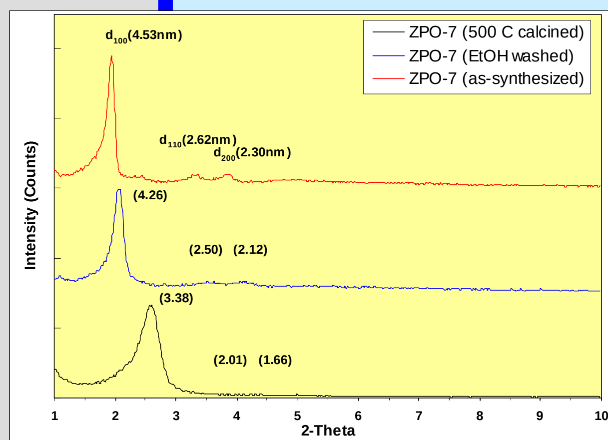
POC: Shas Mattigod

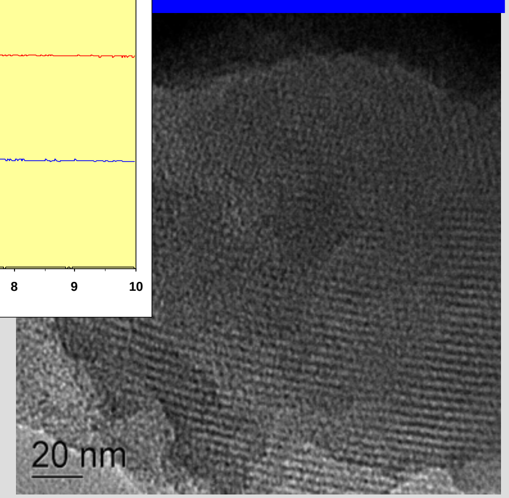
Mesoporous metal phosphates

The major long-term concern at YMP are the actinides (esp. Np), as well as radioiodine and Tc-99.

- Mesoporous metal phosphates are inherently bifunctional (i.e. can bind both anions and cations)
- Maximize functional density while maintaining an open pore structure
- Literature precedent indicates that these materials are inherently cationic and have high anion exchange capacities.
- Structurally, they should be well-suited for TcO4- sequestration, as well as actinides







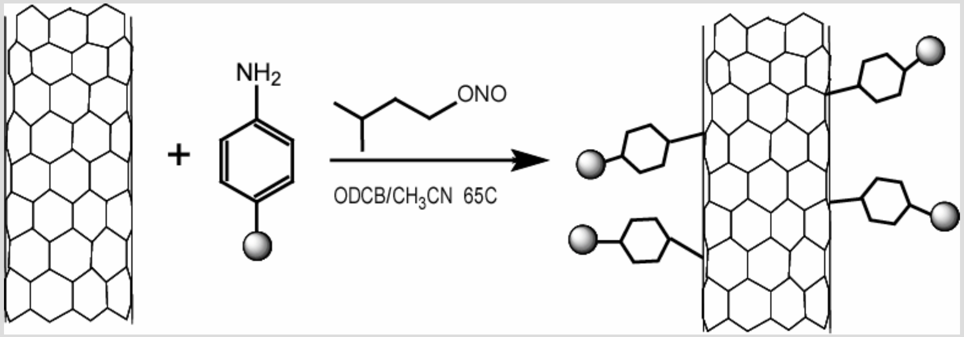
$Zr_3(PO_4)_4$

Pore size – 28-65Å
Surface area – 400-700 m2/g
Anion capacities – 4.7-5.4 mmole/g

POC: Shas Mattigod

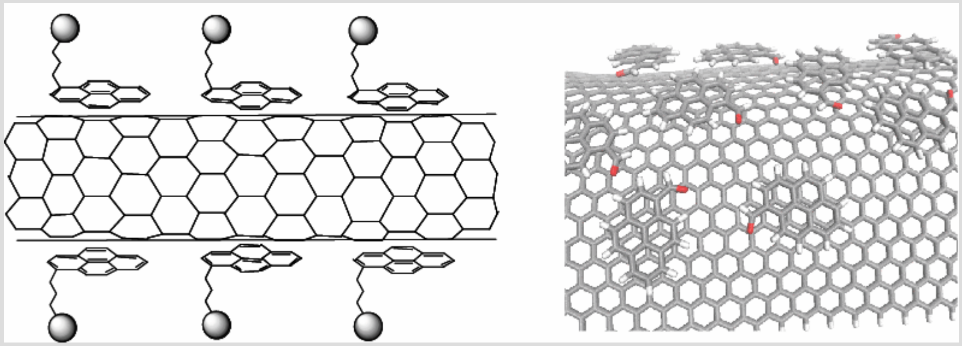
Chemically Modified Carbon Nanotubes

CNT's have high thermal and electrical conductivity and can be used for selective and reversible sorption.



There are two strategies being used to chemically modify CNT's:

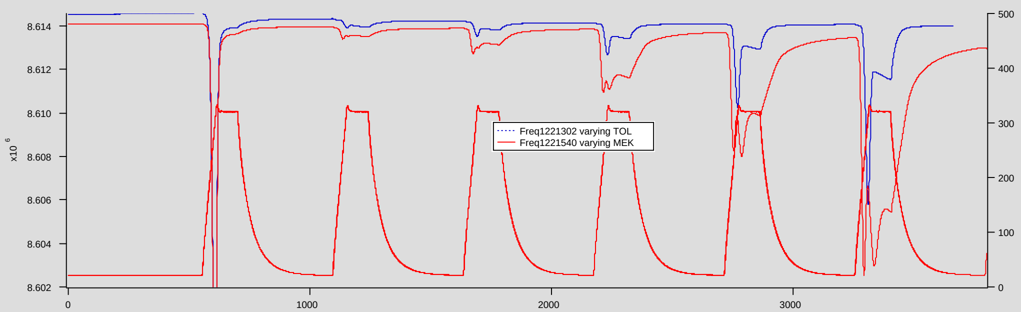
Covalent and non-covalent functionalization

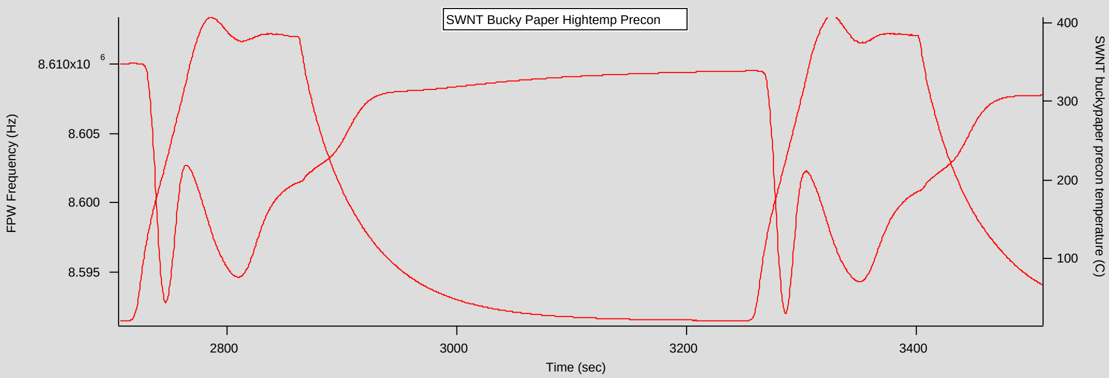


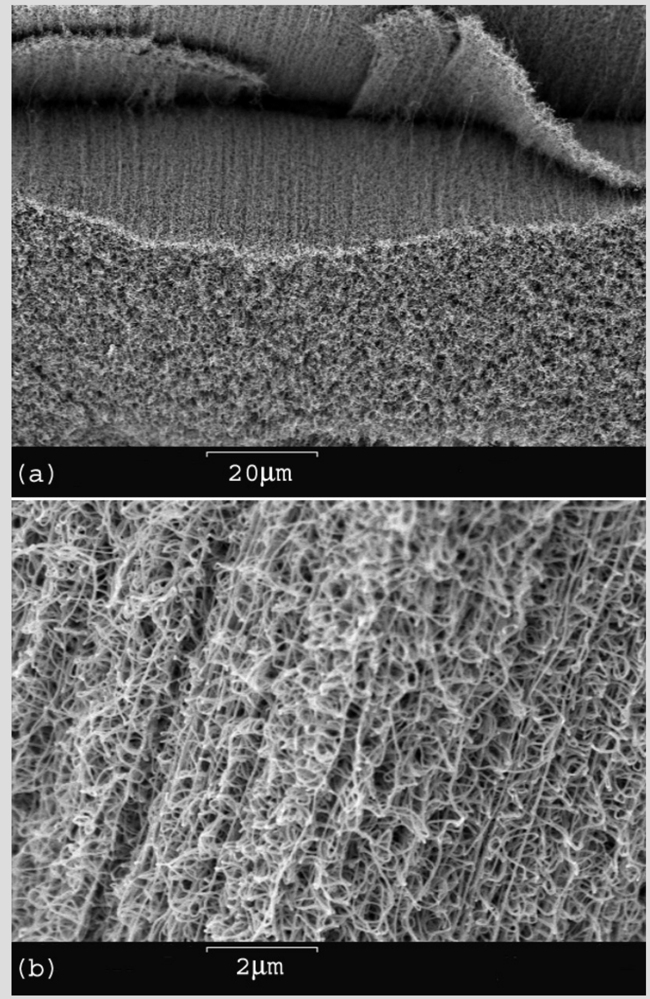
These functional CNT's are being studied for preconcentration of organic signature compounds, heavy metals, radionuclides and CO_2

Preconcentration of Organic Signatures on Carbon Nanotube Composites

Preconcentrator Test -- Sensor Array







CNT's can serve as highly effective, and reversible, sorbent materials for preconcentration.

POC: Chris Aardahl

Fe and Fe-oxide Nanoparticles

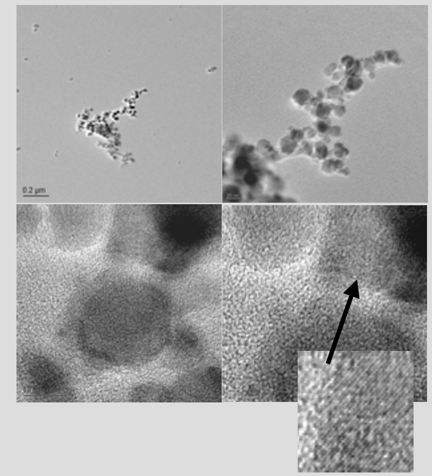
Useful as an *in situ* reductant for DNAPL's, chromate, etc.

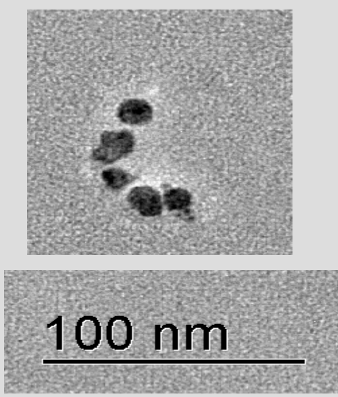
What do we need to know about Fe and Fe-oxide nanoparticles to understand their chemical properties?

What properties of iron nanoparticles change the reaction path and why?

Find appropriate ways to make, handle and characterizing the Fe and Fe-Oxide nanoparticles.

RESS grown particles

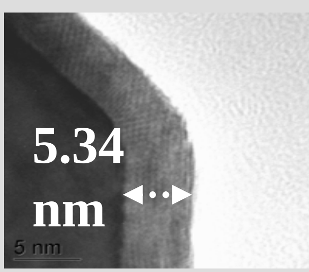




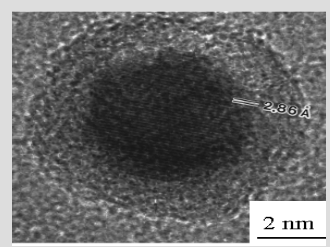
Fe(CO)5

Unlike vacuum studies of supposedly inert materials, we are interested in the behavior and characterization of reactive metals in an aqueous environment.

Oxide covered Fe(0) iron surface



Magnetron Sputtering



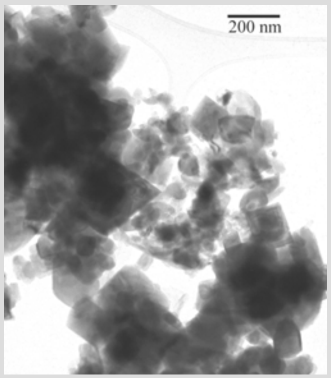
POC: Don Baer

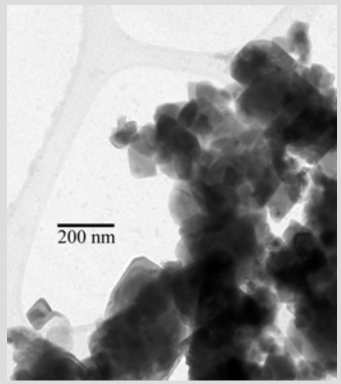
Battelle

Pacific Northwest National Laboratory
U.S. Department of Energy

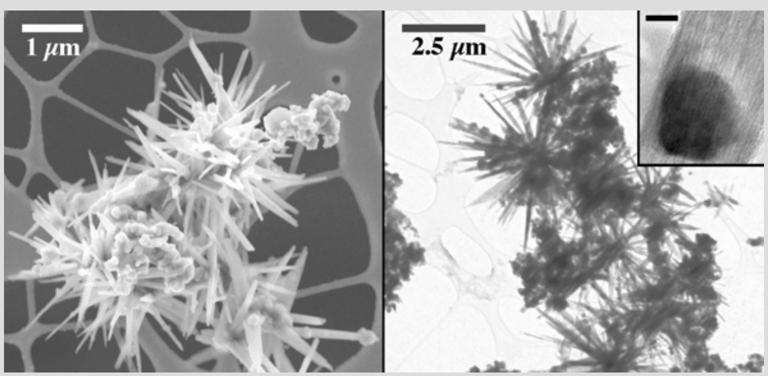
Behavior of Fe and Fe-oxide nanoparticles

Suspending the particles in a solution of TTAB results in a predominantly magnetite(or maghemite) particles.



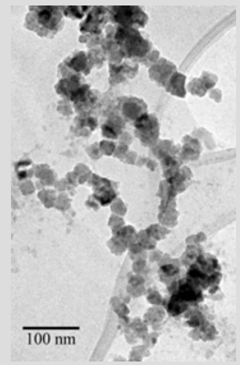


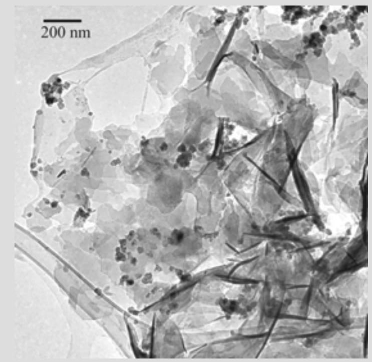
Suspending the particles in water results in mostly lepidocrocite spicules and some magnetite particles, which are often attached to the spicules.

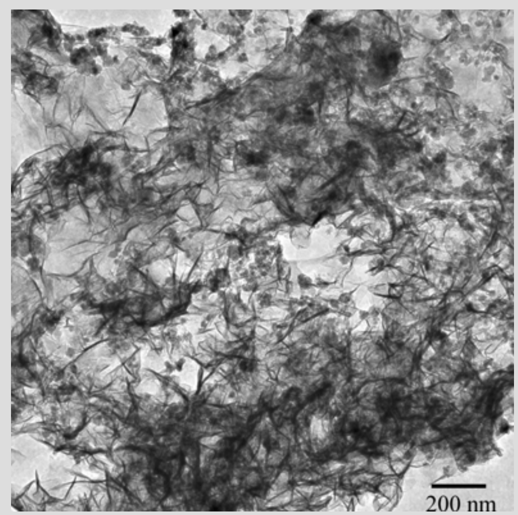


Toda

Suspending the particles in a solution of TTAB results in a heterogeneous mixture of magnetite, lepidocrocite (crumpled sheet morphology).







Suspending the particles in water results in mostly lepidocrocite sheets and some magnetite.

Zhang

POC: Don Baer

Nanomaterials Needs

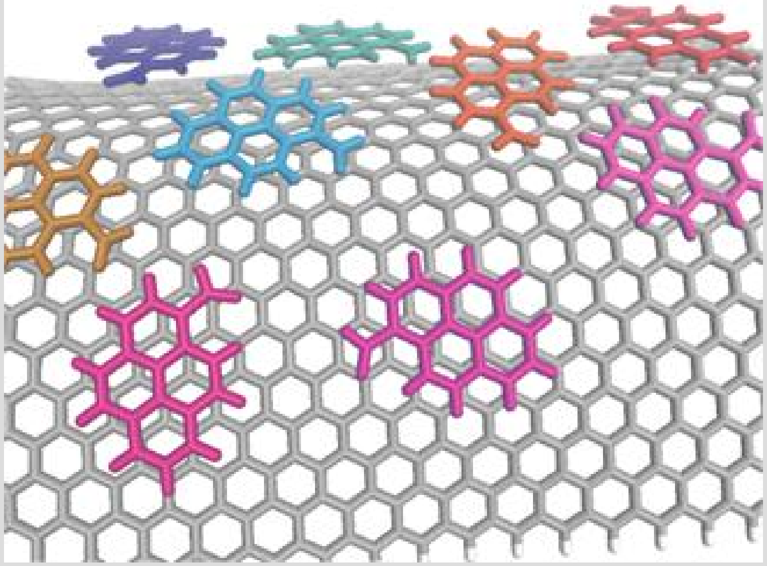
Recently (March 2004), an NIEHS workshop on nanomaterials and the environment concluded:

- Need additional work in the design and synthesis of new nanomaterial phases
- Better understanding of surface reactivity (environment, contaminants, etc.)
- Better understanding of how nanomaterials behave in the environment (mobility, dispersability, bio-fouling, etc.)
- Integration of nanomaterials with existing technology (e.g. nanoparticles into GAC)
- Nanomaterials to empower remote sensing, to support remediation efforts

Nanomaterials for Environmental Remediation

- PNNL research is actively aimed at solving problems associated with contamination from heavy metals, radionuclides, organics, DNAPL's and greenhouse gases.
- Environmental remediation requires *functional* nanomaterials, and the ability to tune functionality
- PNNL is currently developing environmental remediation technologies based on MP ceramics, nanoparticles and CNT's.
- Multiple material foundations allows materials to be tailored for a wide variety of application conditions (both *in situ* and *ex situ*)

CNT's chemically modified through pi-stacking



Path forward – we need :

- Better and more sophisticated characterization tools
- Design and synthesis of new *functional* nanomaterial phases
- Better understanding of how nanomaterials behave in the environment