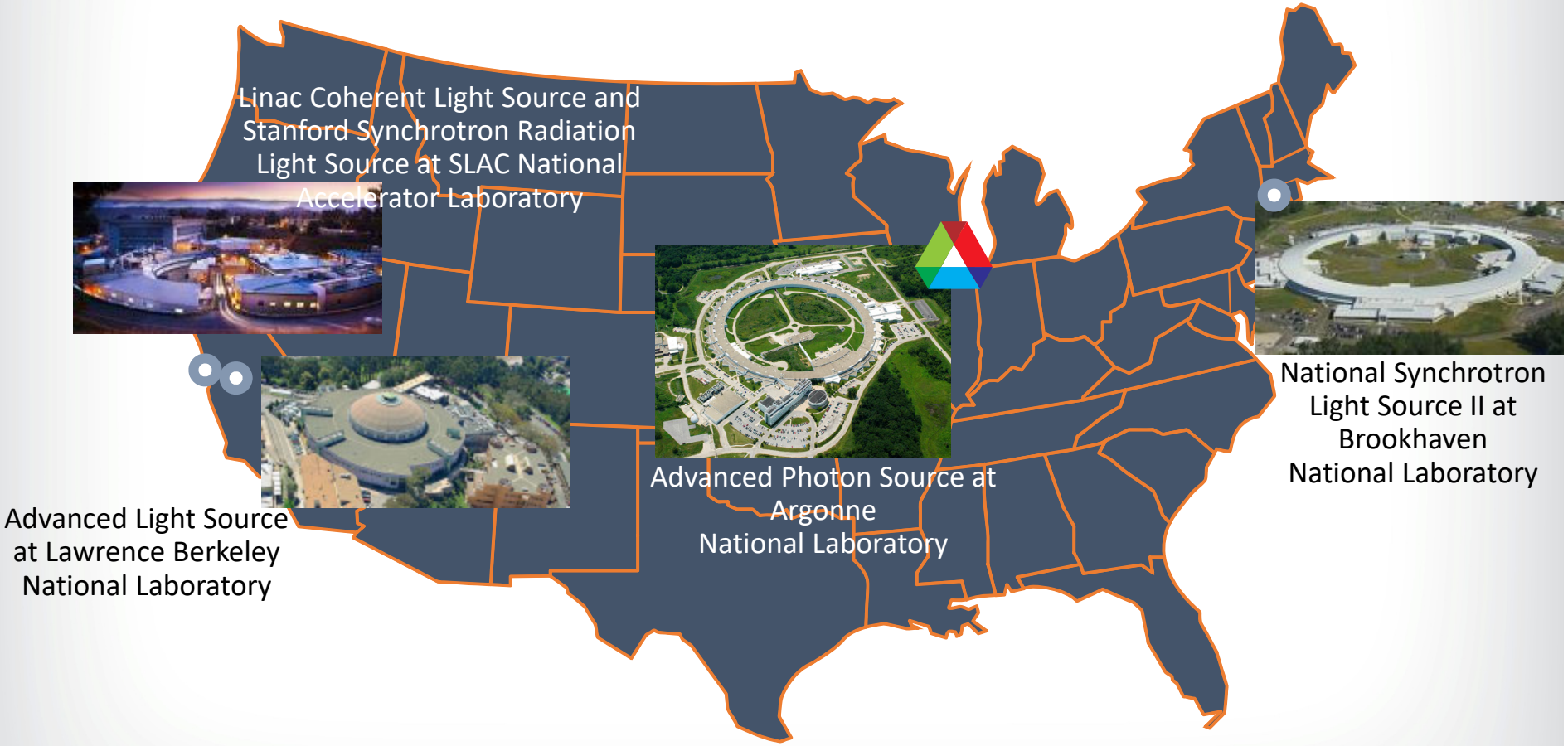
Application of X-ray Absorption Spectroscopy for Monitoring Transformation of Nanomaterials

Kirk Scheckel

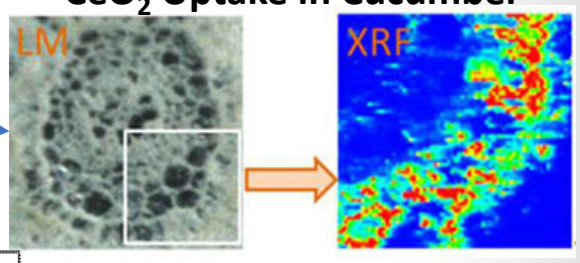
U.S. Department of Energy Office of Science X-ray Light Sources

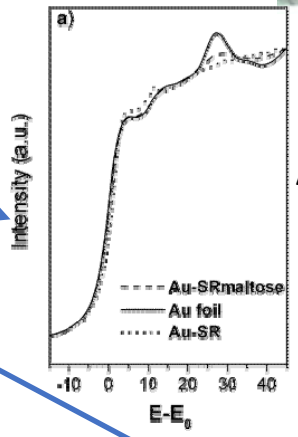


Spectroscopic Transformation of Nanomaterials

- **X-ray Fluorescence (XRF):** chemical composition (quantification, mapping)
- **X-ray Absorption Spectroscopy (XAS):** chemical speciation (oxidation state, coordination, nearest neighbors)
- **Surface Scattering and Diffraction:** surface structure, sorption processes
- **Microtomography:** 3D imaging of internal microstructure (porosity, fluid flow, composition)

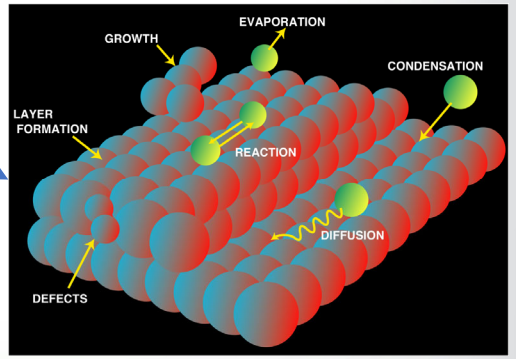
CeO_2 Uptake in Cucumber

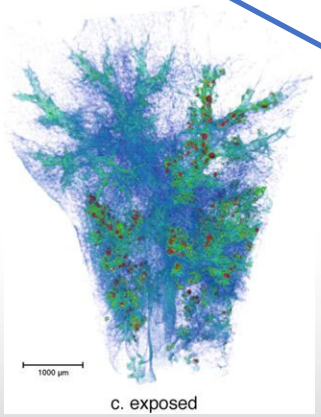




Au NPs with different capping agents

Surface Reactions

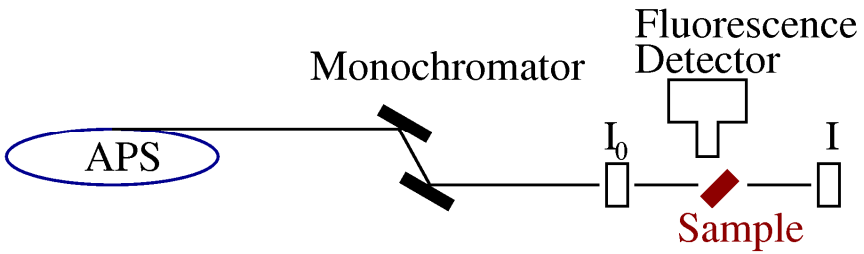


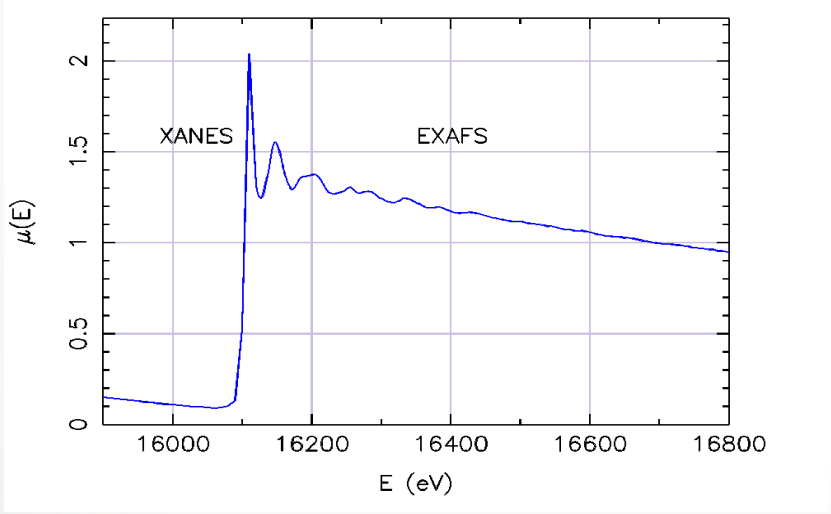


TiO_2 in mouse lung

Spectroscopic Transformation of Nanomaterials

X-ray Absorption Spectroscopy: Measure energy-dependence of the x-ray absorption coefficient μ(E) [either log(I_0 /I) or (I_f / I_0)] of a core-level of a selected element





XANES = X-ray Absorption Near Edge Structure

EXAFS = Extended X-ray Absorption Fine Structure

Element Specific: Elements with Z>20 (5) can be examined.

Valence Probe: XANES gives chemical state and formal valence of selected element.

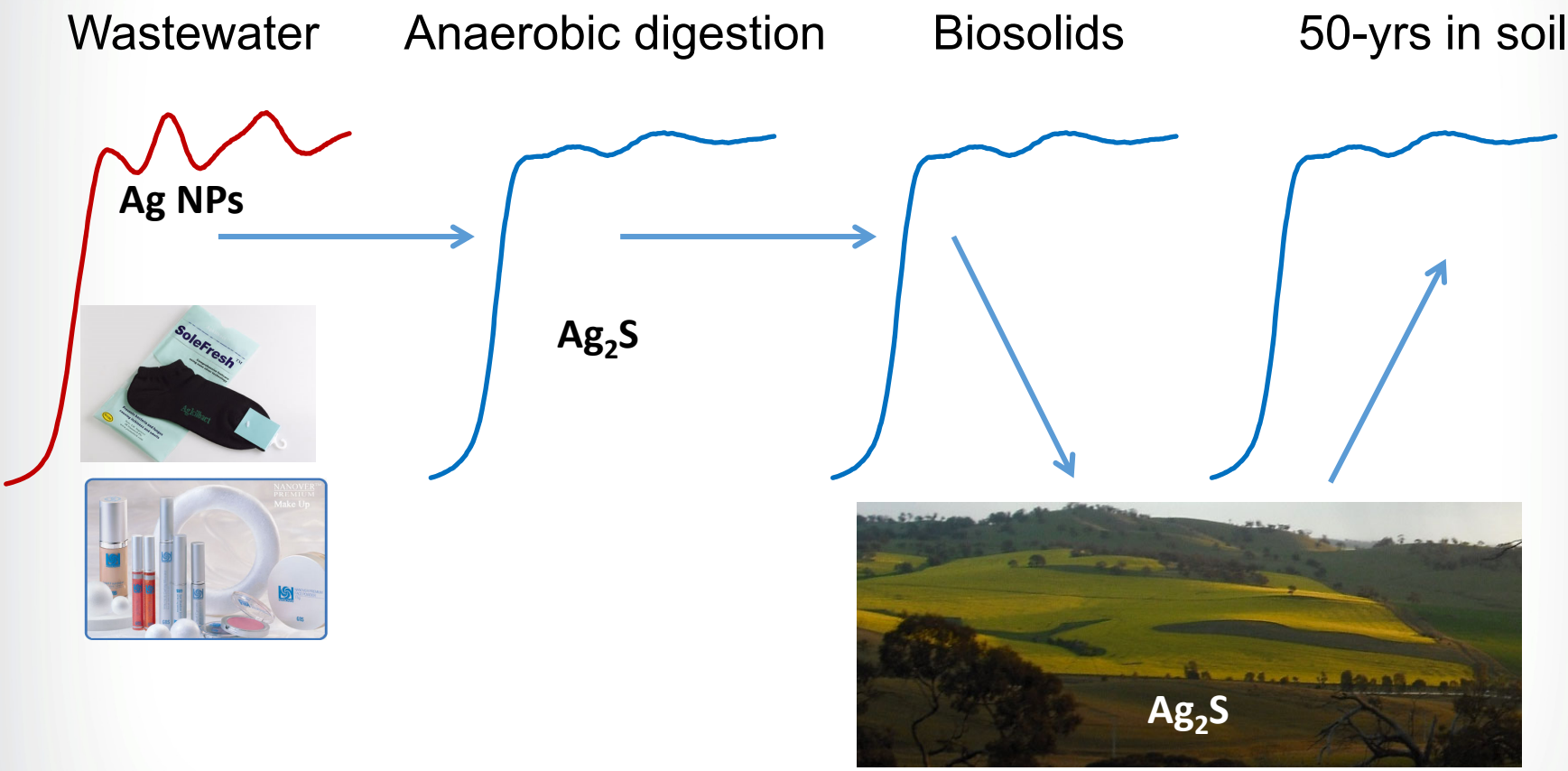
Local Structure Probe: EXAFS gives atomic species, distance, and number of near-neighbor atoms around a selected element..

Low Concentration: concentrations down to 1 ppm for XANES, 10 ppm for EXAFS.

Natural Samples: samples can be in solution, liquids, amorphous solids, soils, aggregates, plant roots, surfaces, etc.

Small Spot Size: XANES and EXAFS measurements can be made on samples down to 50 nm in size.

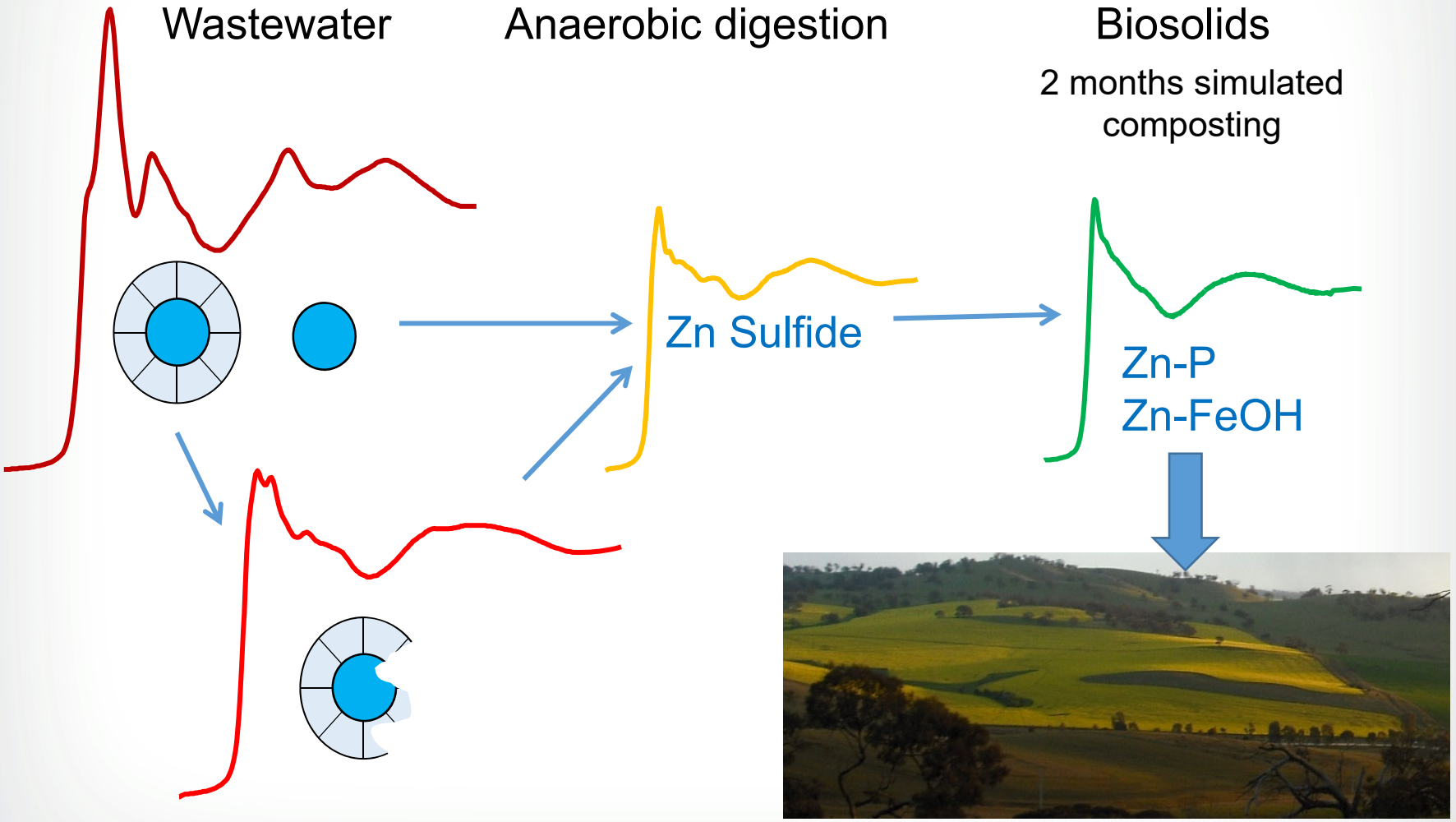
Spectroscopic Transformation of Nanomaterials



Transformation of Four Silver/Silver Chloride Nanoparticles during Anaerobic Treatment of Wastewater and Post-processing of Sewage Sludge. E. Lombi, E. Donner, S. Taheri, E. Tavakkoli, Å. Jamting, S. McClure, R. Naidu, B.W. Miller, K.G. Scheckel and K. Vasilev. 2013. Environ. Pollut. 176: 193-197.

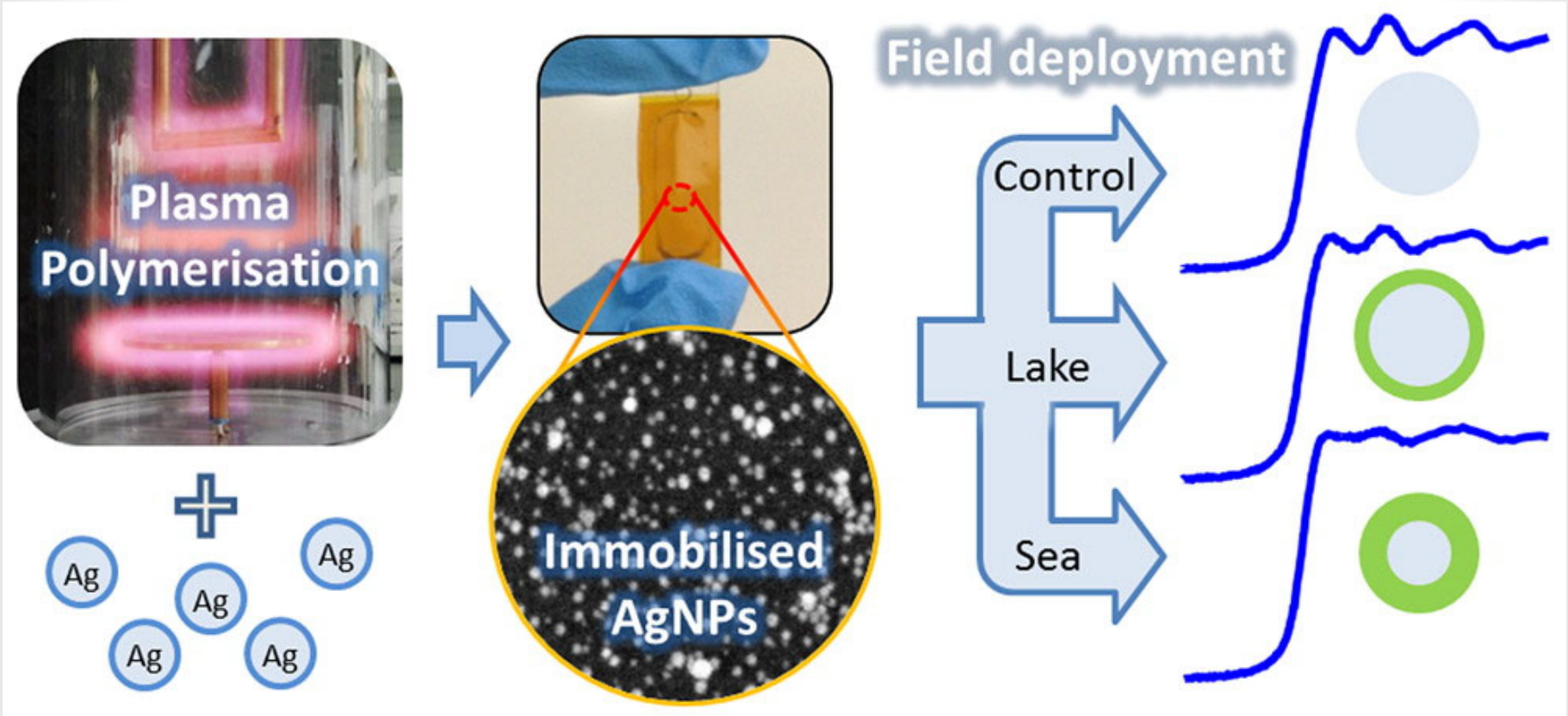
Non-labile Silver Species in Biosolids remain Stable throughout 50 Years of Weathering and Ageing. E. Donner, K.G. Scheckel, R. Sekine, R.S. Popelka-Filcoff, J.W. Bennett, G. Brunetti, R. Naidu, S.P. McGrath, E. Lombi. 2015. Environ. Pollut. 205: 78-86.

Spectroscopic Transformation of Nanomaterials



Fate of Zinc Oxide Nanoparticles during Anaerobic Digestion of Wastewater and Post-treatment Processing of Sewage Sludge. E. Lombi, E. Donner, E. Tavakkoli, T. Turney, R. Naidu, B.W. Miller and K.G. Scheckel. 2012. Environ. Sci. Technol. 46: 9089-9096.

Spectroscopic Transformation of Nanomaterials



Surface Immobilization of Engineered Nanomaterials for in-situ Study of their Environmental Transformations and Fate. R. Sekine, M. Khaksar, G. Brunetti, E. Donner, K.G. Scheckel, E. Lombi and K. Vasilev. 2013. Environ. Sci. Technol. 47: 9308-9316.

Spectroscopic Transformation of Nanomaterials

The Advanced Photon Source (APS) at the U.S. Department of Energy Office of Science's Argonne National Laboratory provides this hemisphere's most brilliant high-energy x-ray beams for research in almost all scientific disciplines.

Spectroscopic Transformation of Nanomaterials

- Orders of magnitude higher brilliance than tube source
- Translates into major improvements in sensitivity and spatial resolution for x-ray analyses
- Makes some spectroscopic techniques (XAFS) feasible