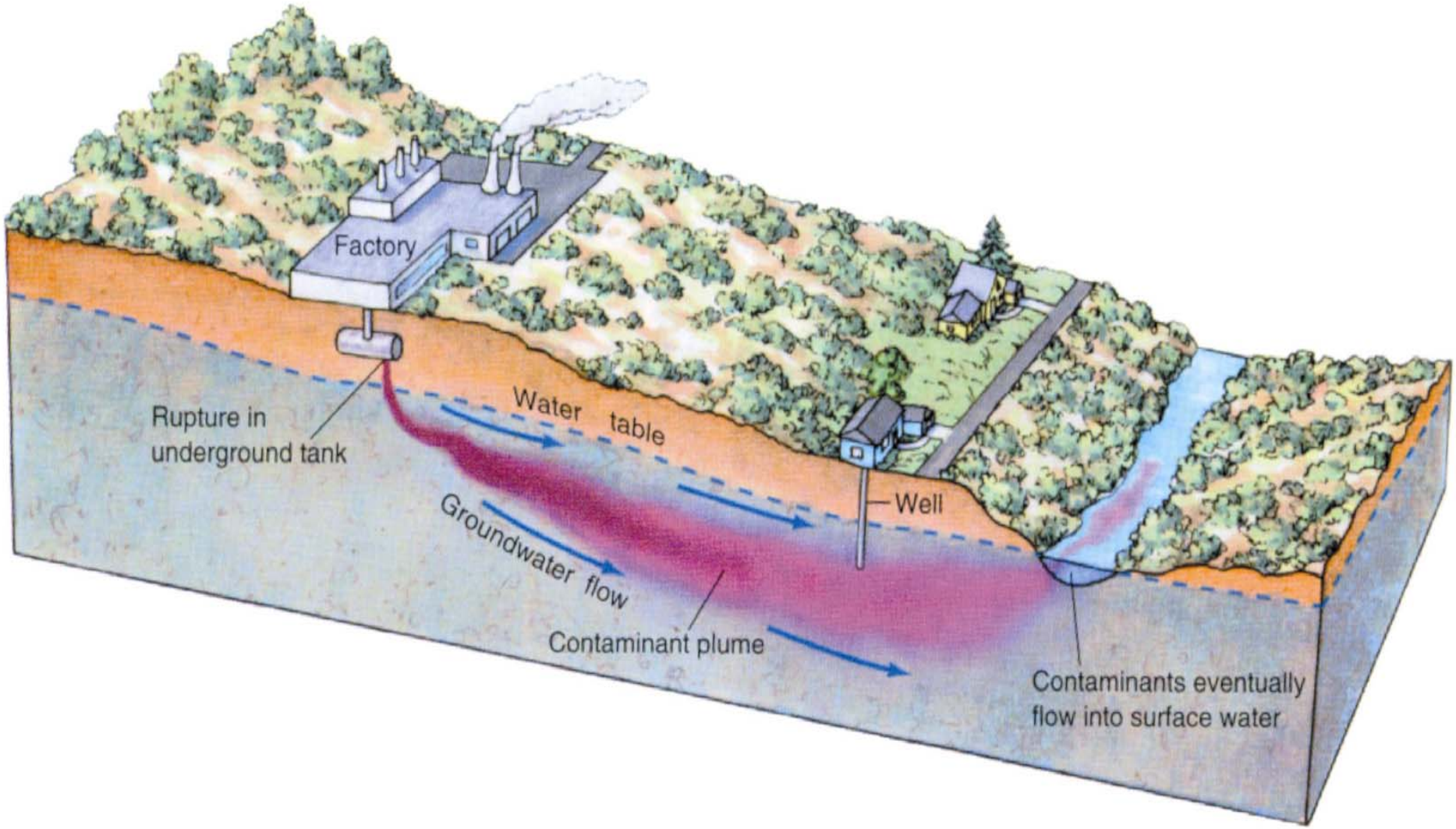
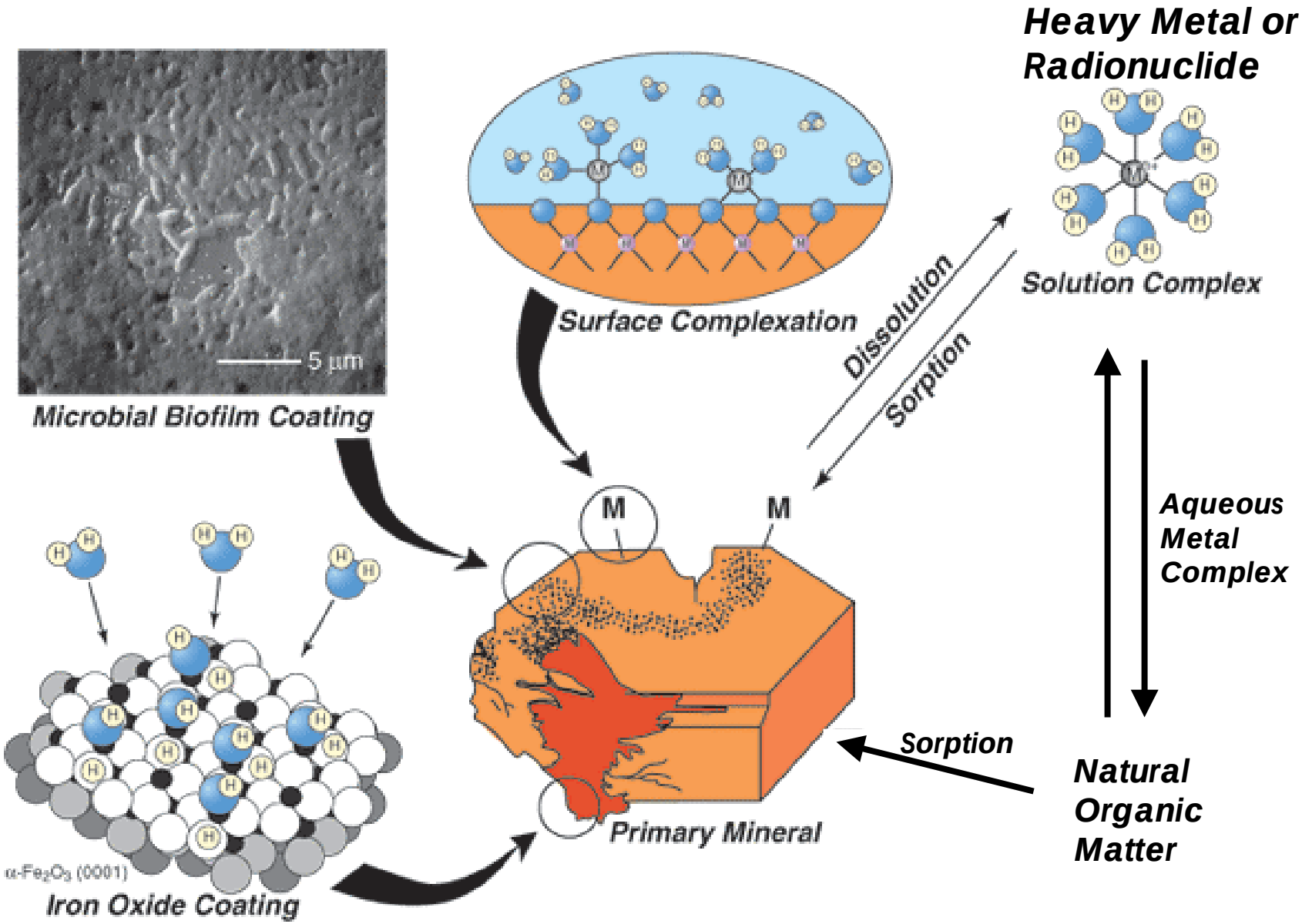
Environmental Molecular Science Institute
University of Notre Dame

Actinides and Heavy Metals in the Environment
The Formation, Stability, and Impact of
Nano- and Micro-Particles

Principal Investigators:
Jeremy Fein, Peter Burns, Patricia Maurice

Civil Engineering and Geological Sciences


Factory
Rupture in
underground tank
Water table
Well
Groundwater flow
Contaminant plume
Contaminants eventually
flow into surface water



After Brown (2003)

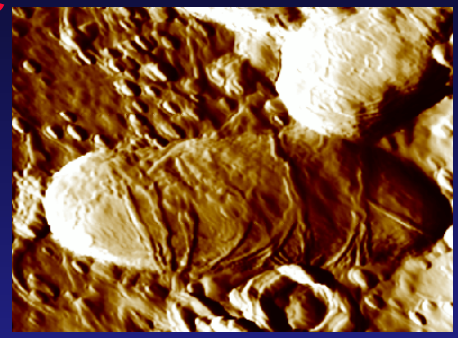
Background:

In order to clean up contaminated groundwater, and to plan for effective geologic disposal of nuclear waste, we must obtain a thorough understanding of the molecular-scale processes that control movement of contaminants in the subsurface.

Scientific Objective:

To determine the effects of bacteria, natural organic matter and other nano- to micro-scale particles on heavy metal (e.g., Cd, Cu, Pb) and actinide (e.g., U, Np) mobilities in groundwater.

Environmental Molecular Science Institute at the University of Notre Dame



Science/Engineering Projects

***Mission*: Determine the effects of nano- and micro-particles on heavy metal and radionuclide transport in geologic systems.**

-Bacteria
-Natural Organic Matter
-Nanoscale Mineral Aggregates

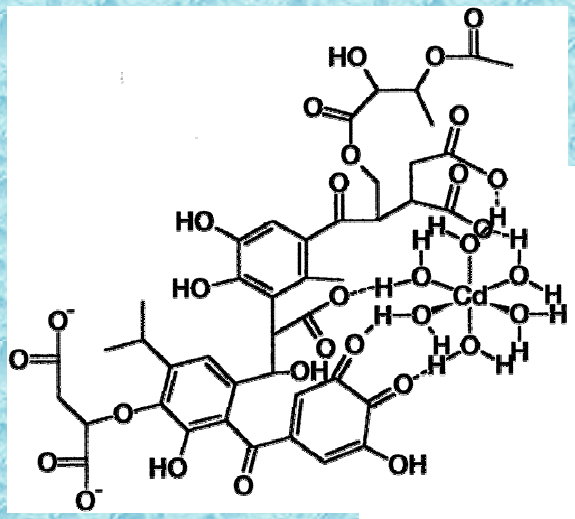
National Lab/Industry Partnerships

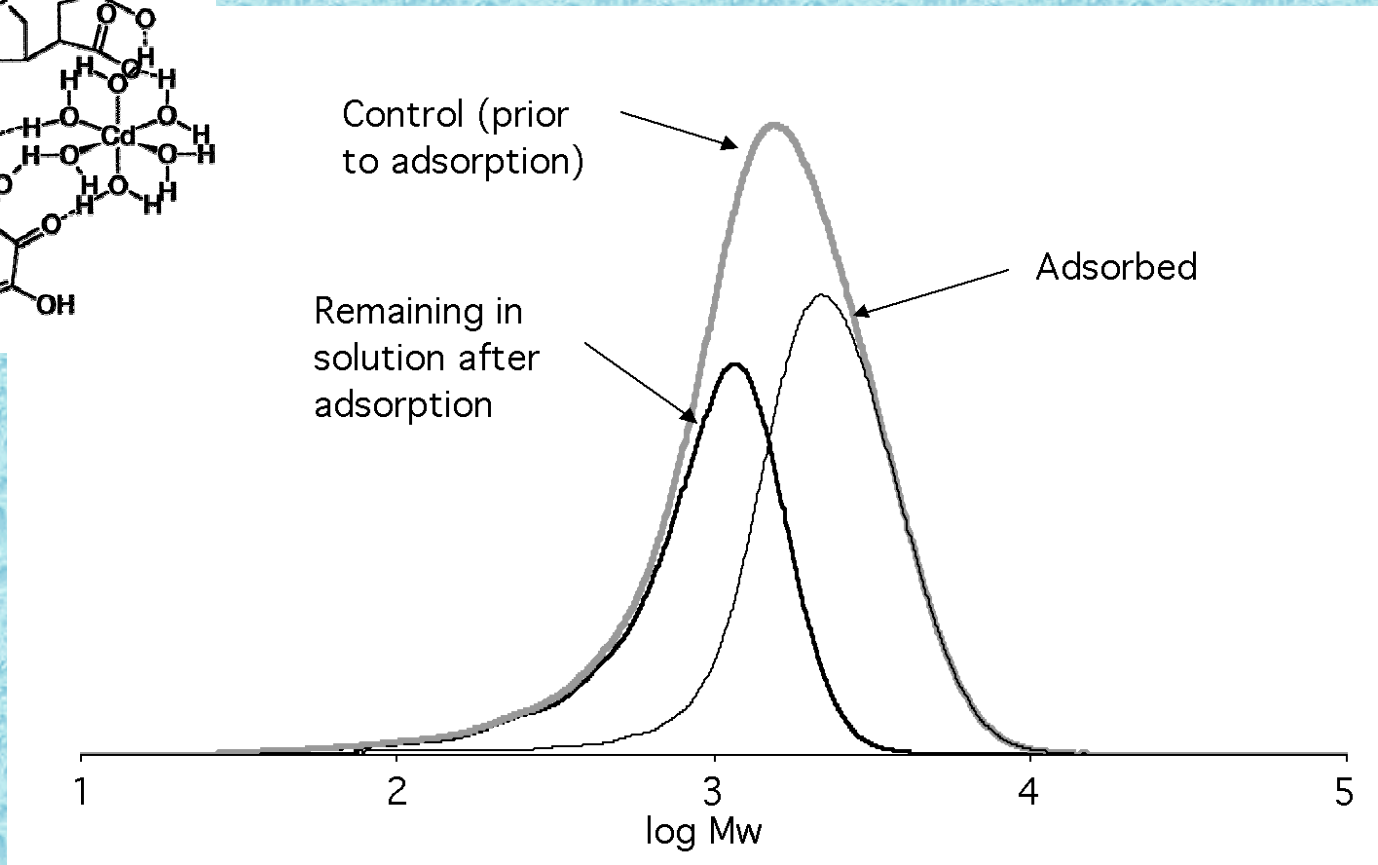
- Argonne (APS; Actinide Facility)
- Sandia (molecular dynamics modeling)
- Oak Ridge (geomicrobiology)
- DuPont Engineering Technologies

Education/Outreach Projects

- REU Summer Program
- High School Student Internships
- Active Recruitment of Under-represented Groups with G.E.M.
- National Lab/Industry Internships

Fulvic/Humic Acid Adsorption and Metal Complexation Reactions

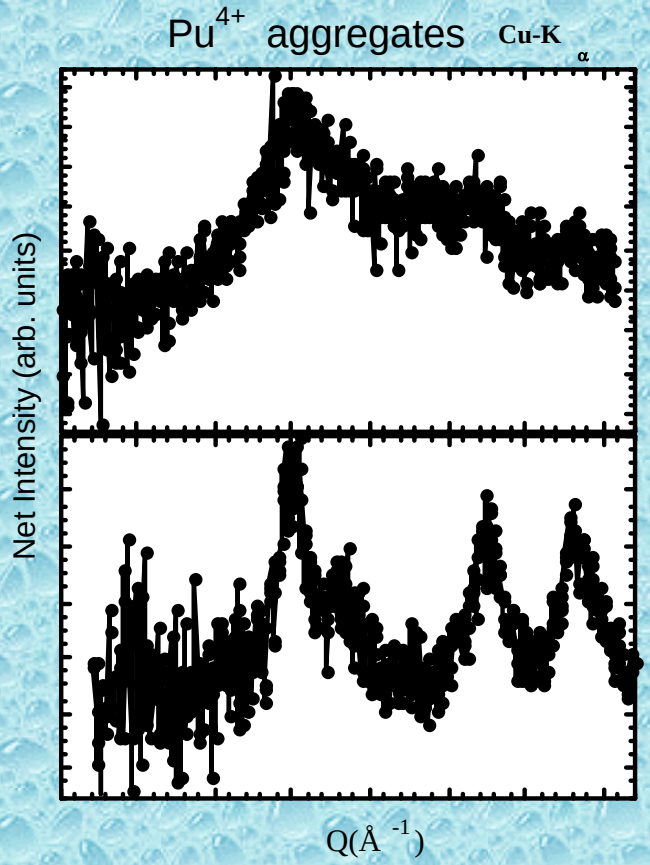




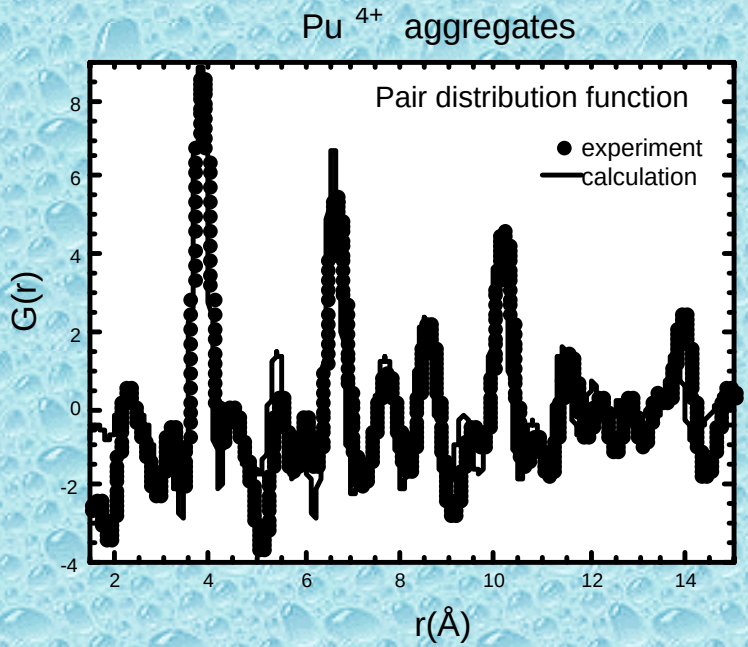
Maurice et al. (2003)

Nano-scale Mineral Aggregates

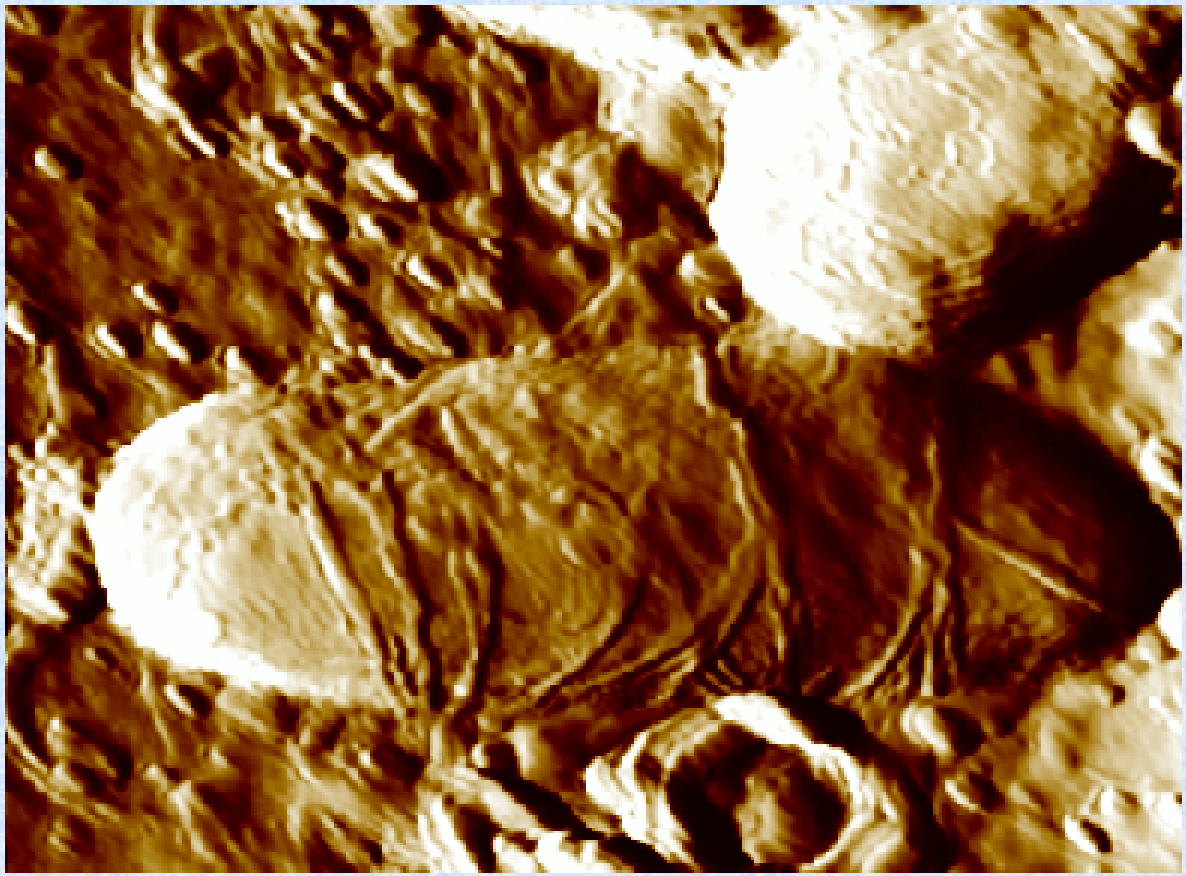
‘Old’ View
Standard X-ray Diffraction

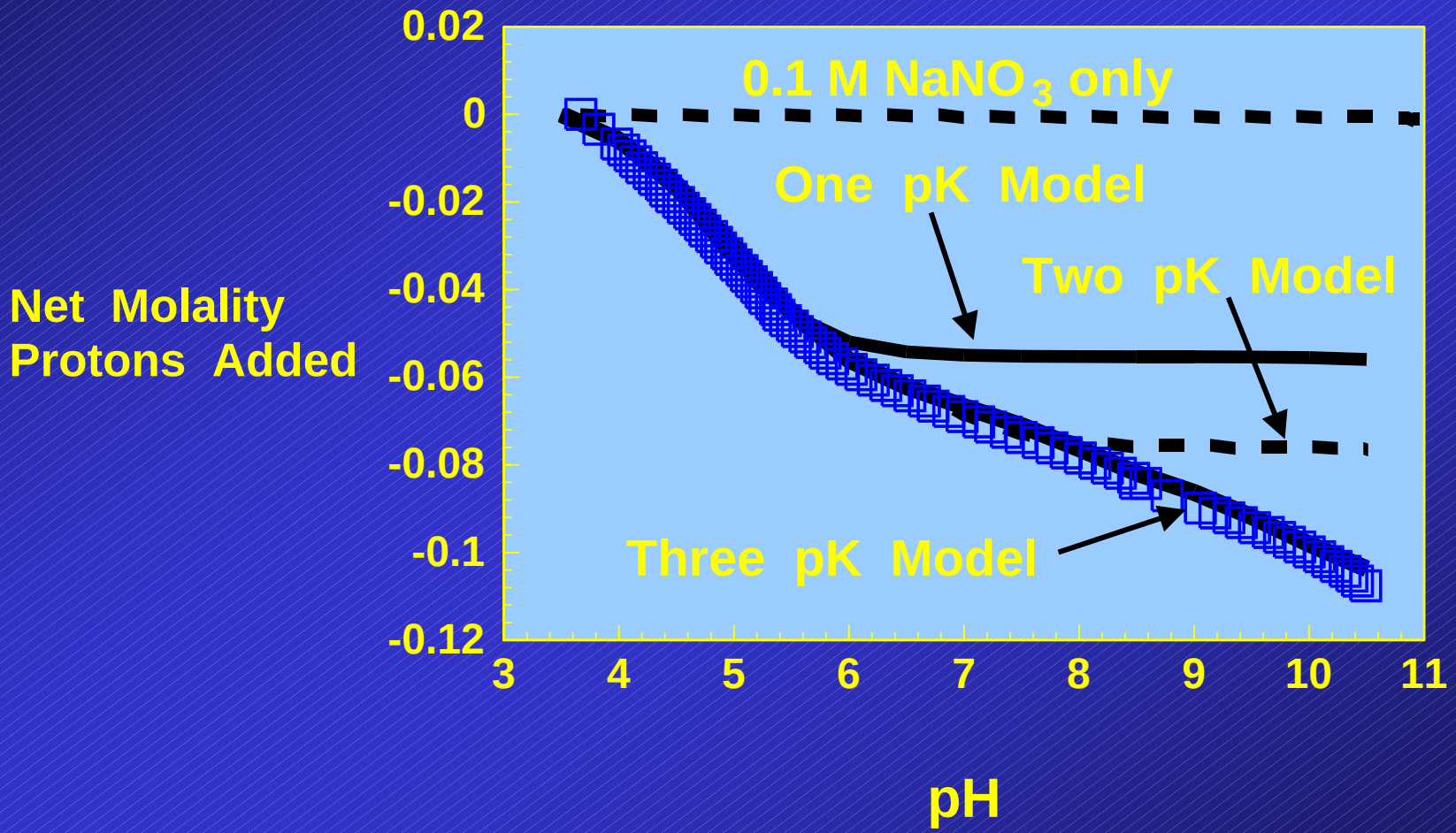


‘New’ View
Advanced Photon Source
X-ray Scattering Data



Bacteria-Contaminant Interactions



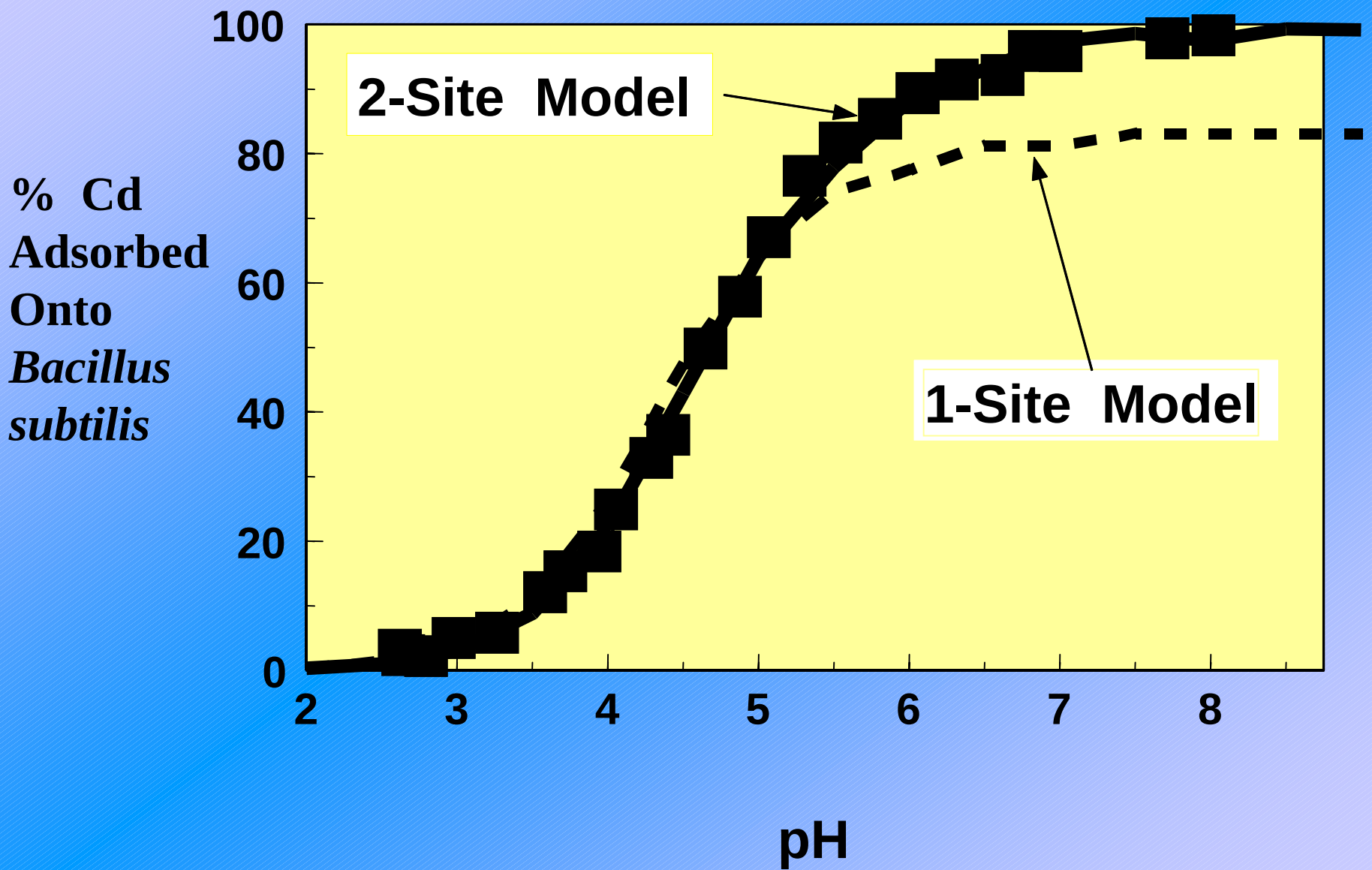

Net Molality
Protons Added
0.02
0
-0.02
-0.04
-0.06
-0.08
-0.1
-0.12
3
4
5
6
7
8
9
10
11
pH
0.1 M NaNO3 only
One pK Model
Two pK Model
Three pK Model

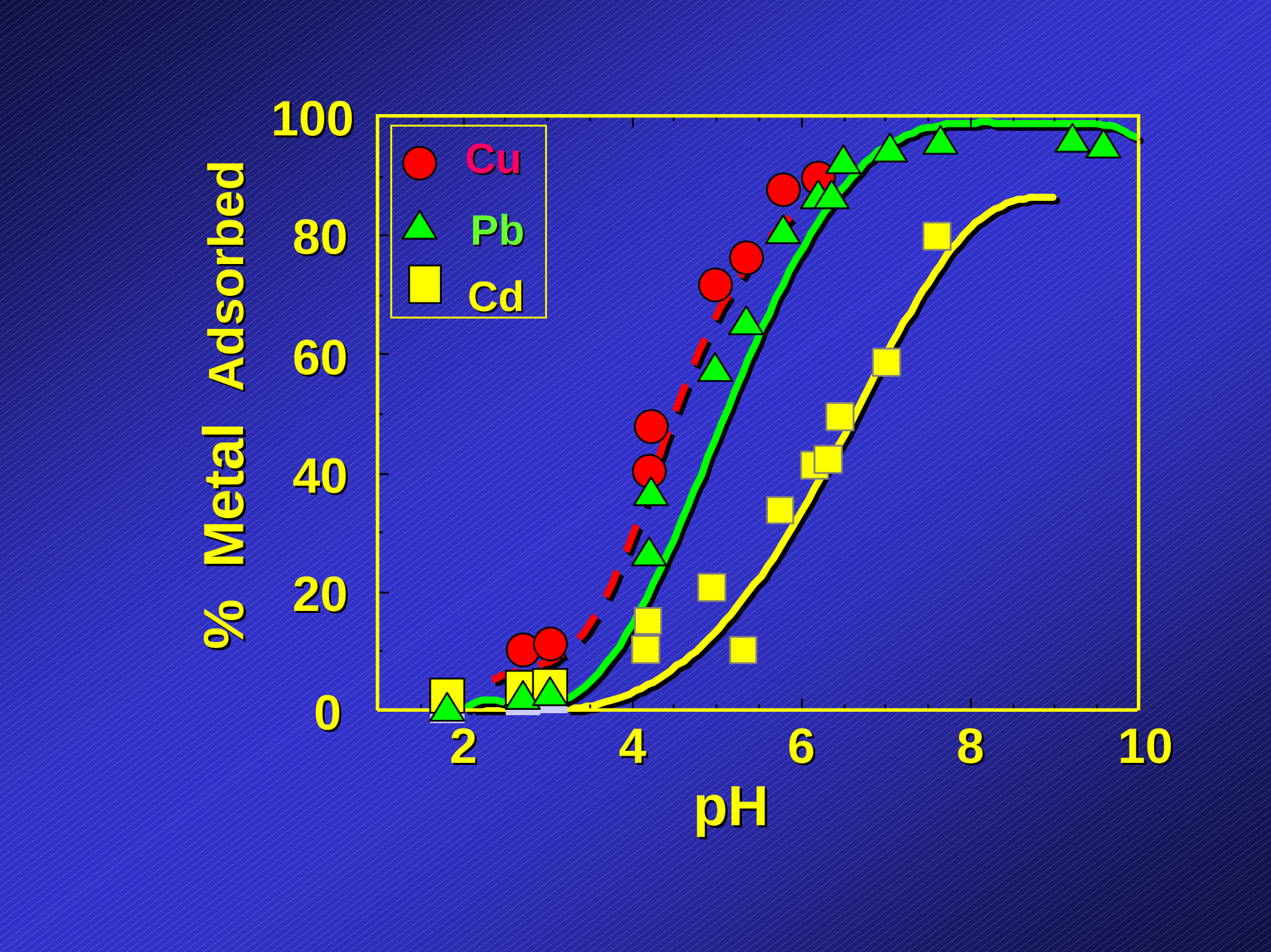
Bacterial Cell Wall Reactions

$R\text{-}COOH^{o} = R\text{-}COO^{-} + H^{+}$ **pKa = 4.8**

$R\text{-}POH^{o} = R\text{-}PO^{-} + H^{+}$ **pKa = 6.9**

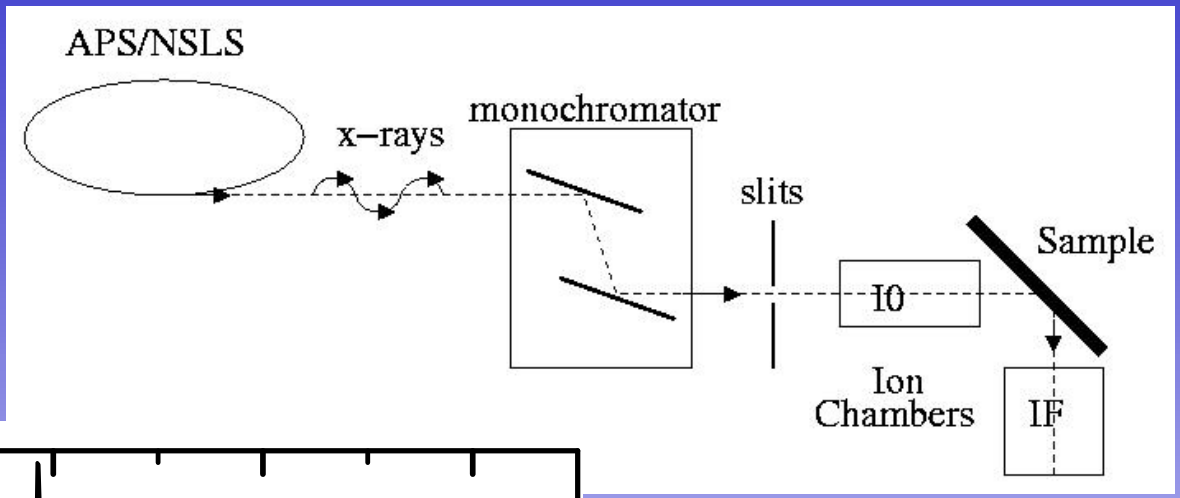
$R\text{-}OH^{o} = R\text{-}O^{-} + H^{+}$ **pKa = 9.4**

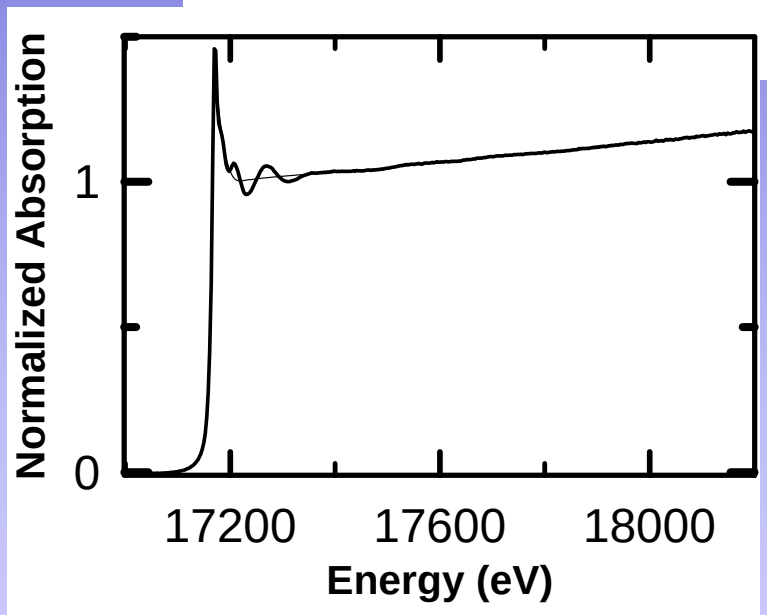

% Cd Adsorbed Onto *Bacillus subtilis*
100
80
60
40
20
0
2
3
4
5
6
7
8
pH
2-Site Model
1-Site Model


% Metal Adsorbed
100
80
60
40
20
0
2
4
6
8
10
pH
Cu
Pb
Cd

Advanced Photon Source
Argonne National Laboratory

X-ray Absorption Fine Structure





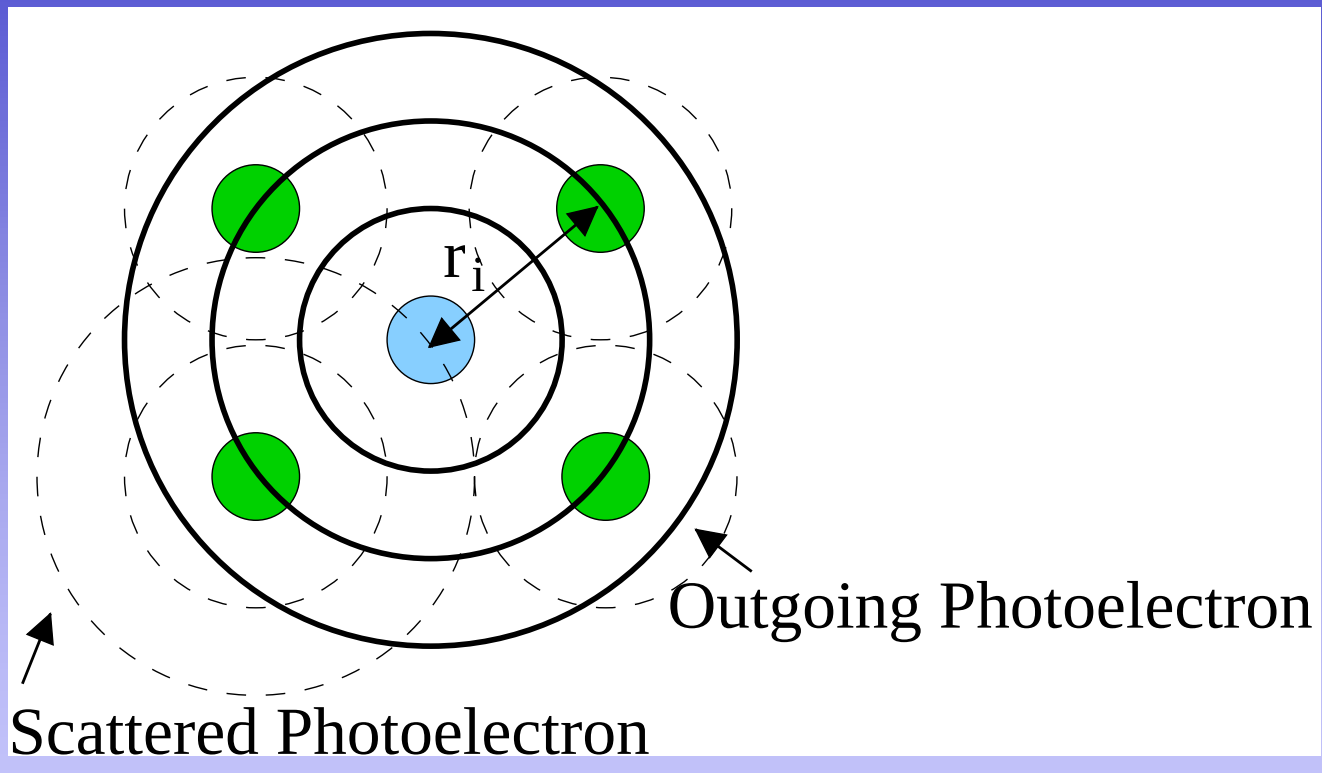
- Attenuation of x-rays

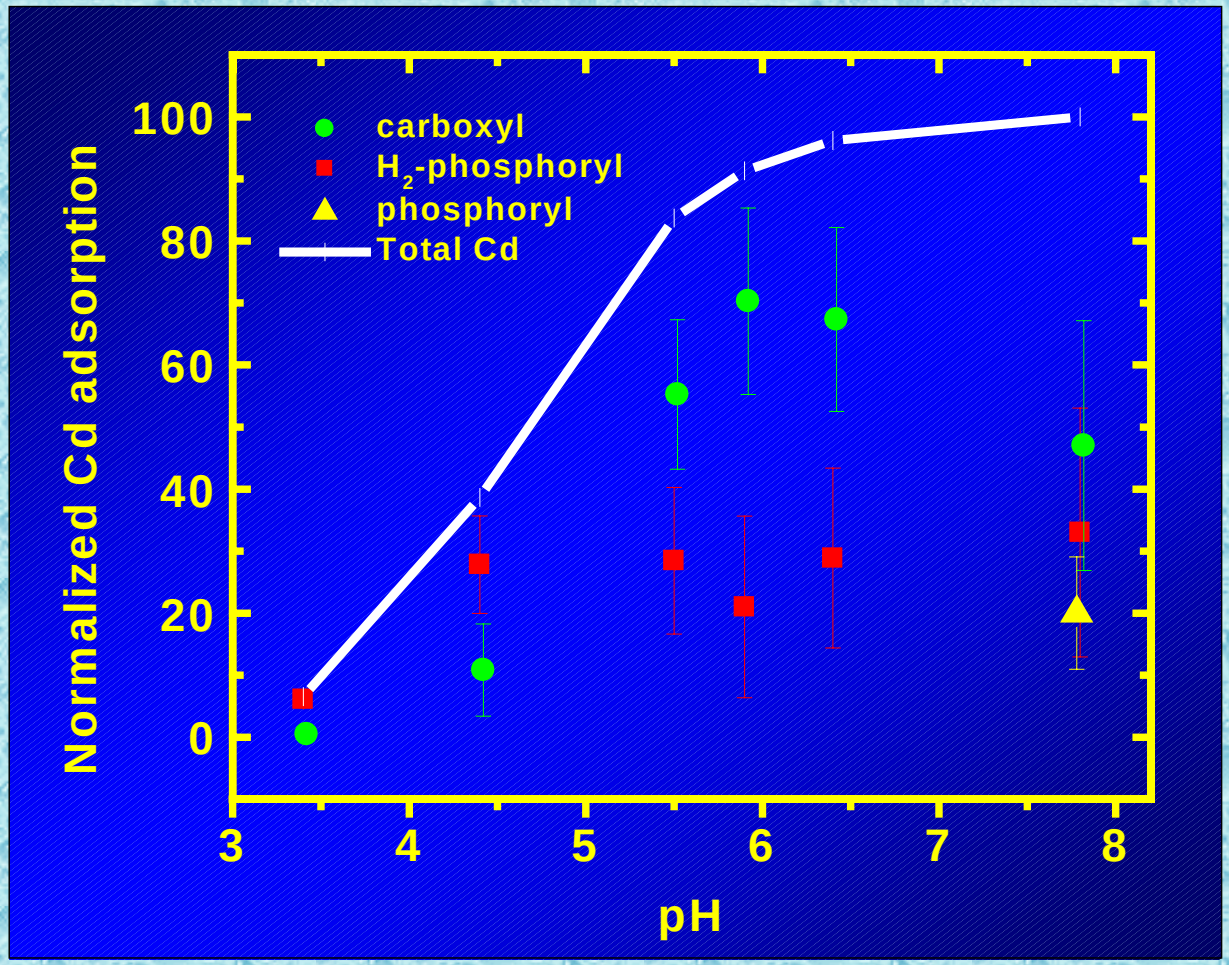
$$I_t = I_0 e^{-\mu(E)\cdot x}$$

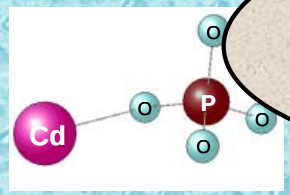
- Absorption coefficient

$$\mu(E) \propto I_f / I_0$$

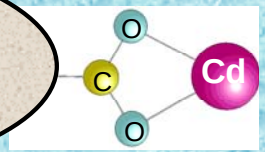
X-ray-Absorption Fine Structure



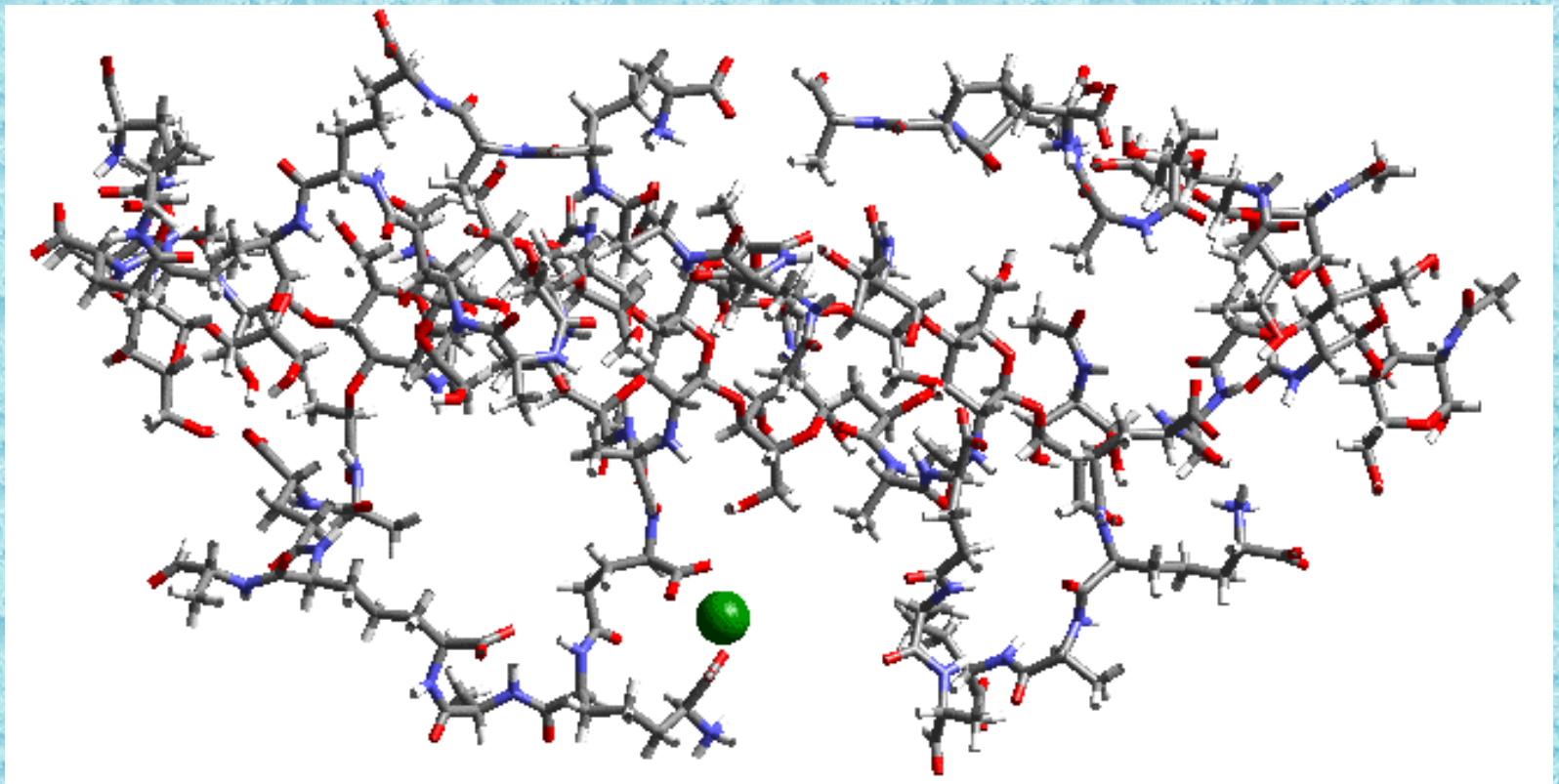




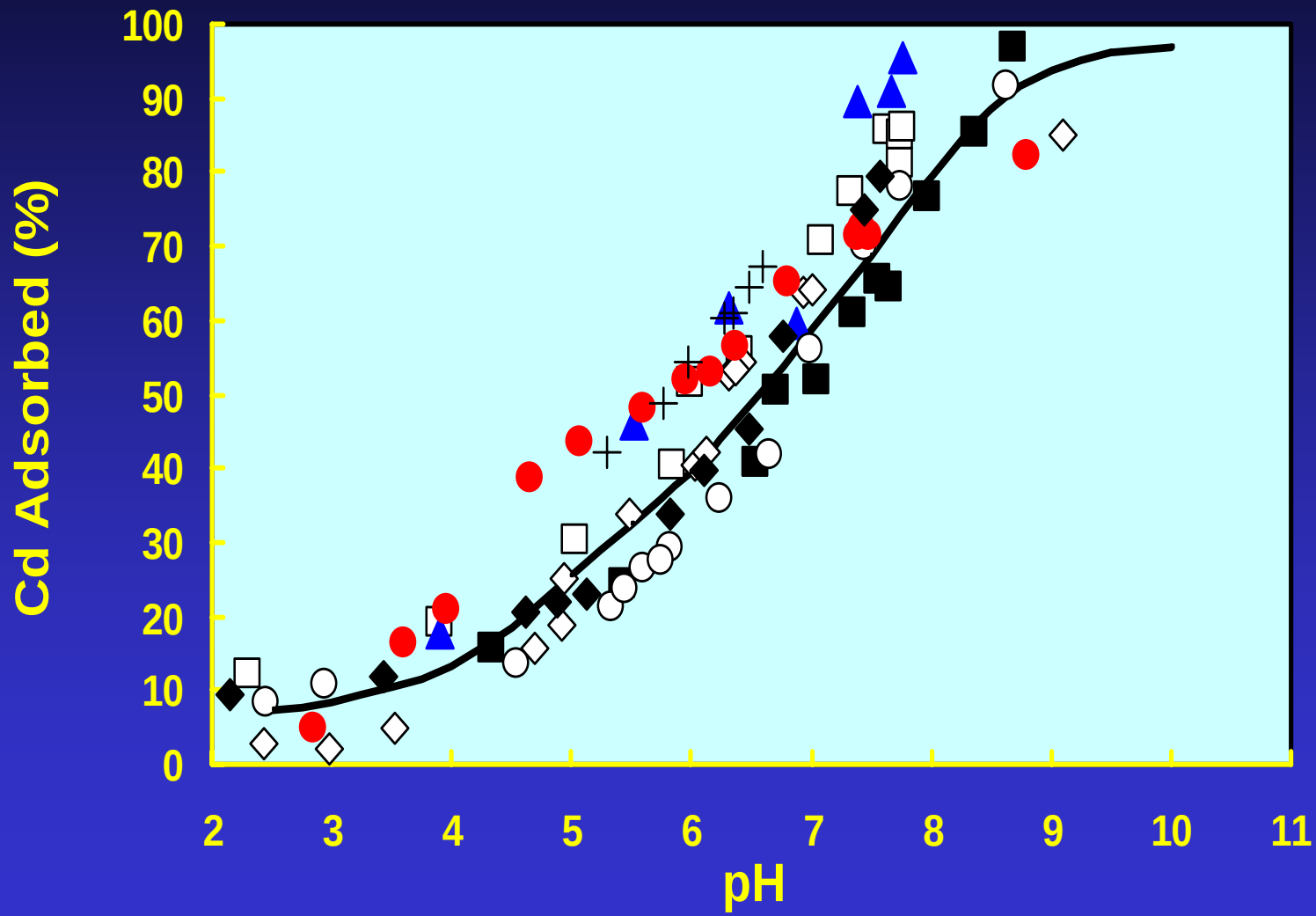
Bacterial surface
5 μm x 1 μm, 140 m^2 /g cell



Molecular Modeling of Metal Binding to Cell Wall Components



Cd Adsorption onto Natural Bacterial Consortia



Conclusions:

- **Nano- and micro-particles can control heavy metal and radionuclide mobilities in the environment.**

- **A range of experimental, analytical, and modeling approaches are required in order to understand the molecular-scale processes that involve these particles.**