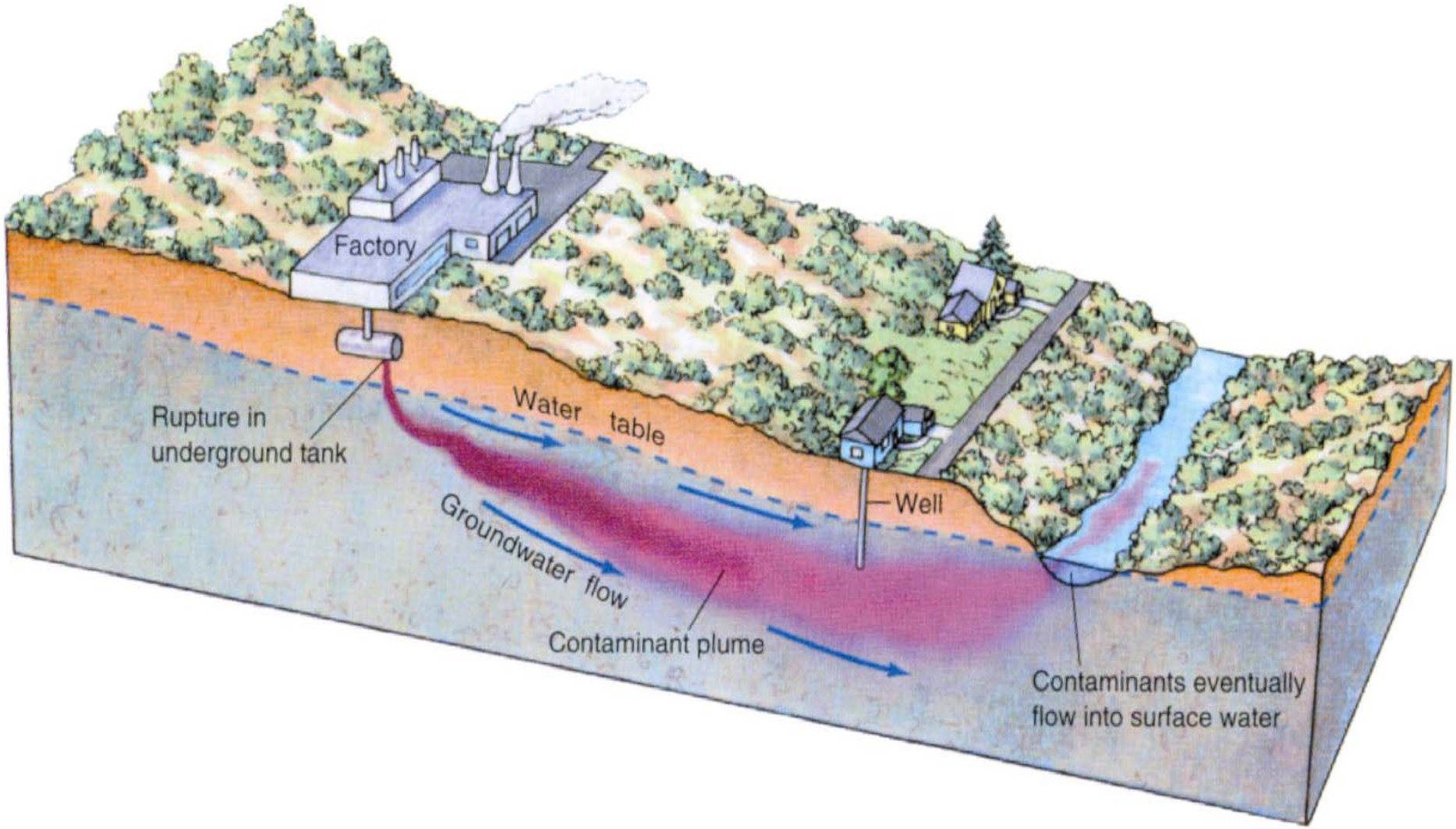
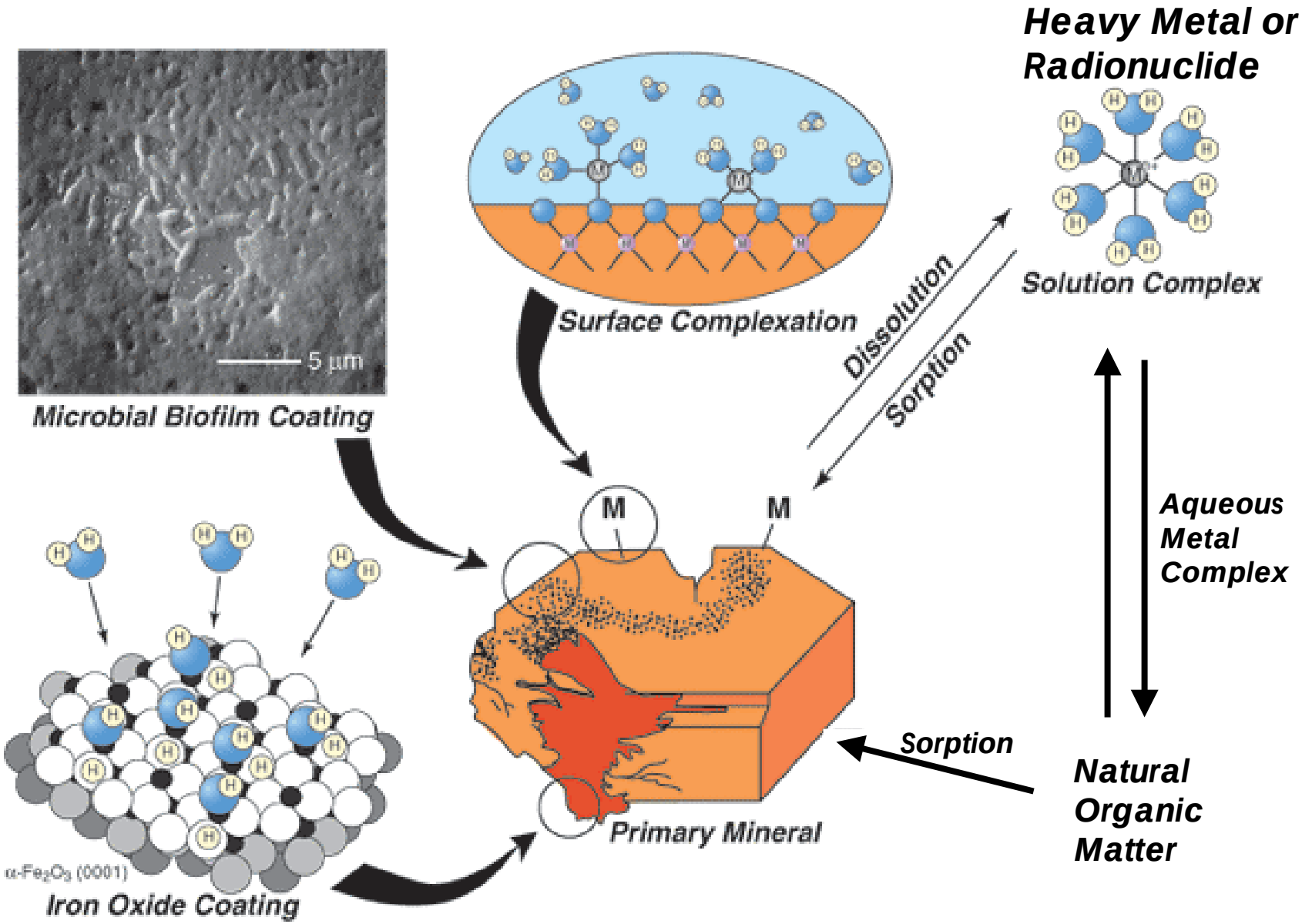
# Environmental Molecular Science Institute
# University of Notre Dame

## 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)*

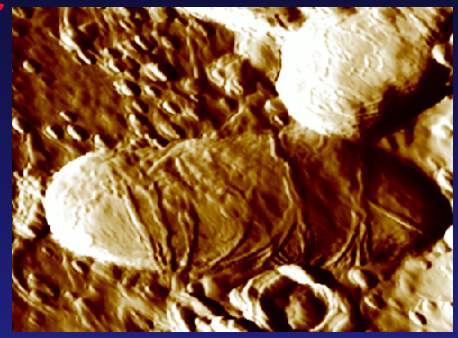
# *Background:*

**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

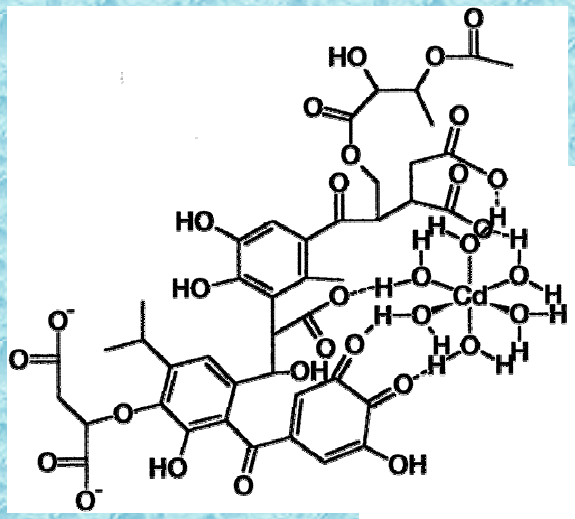
## ***National Lab/Industry Partnerships***

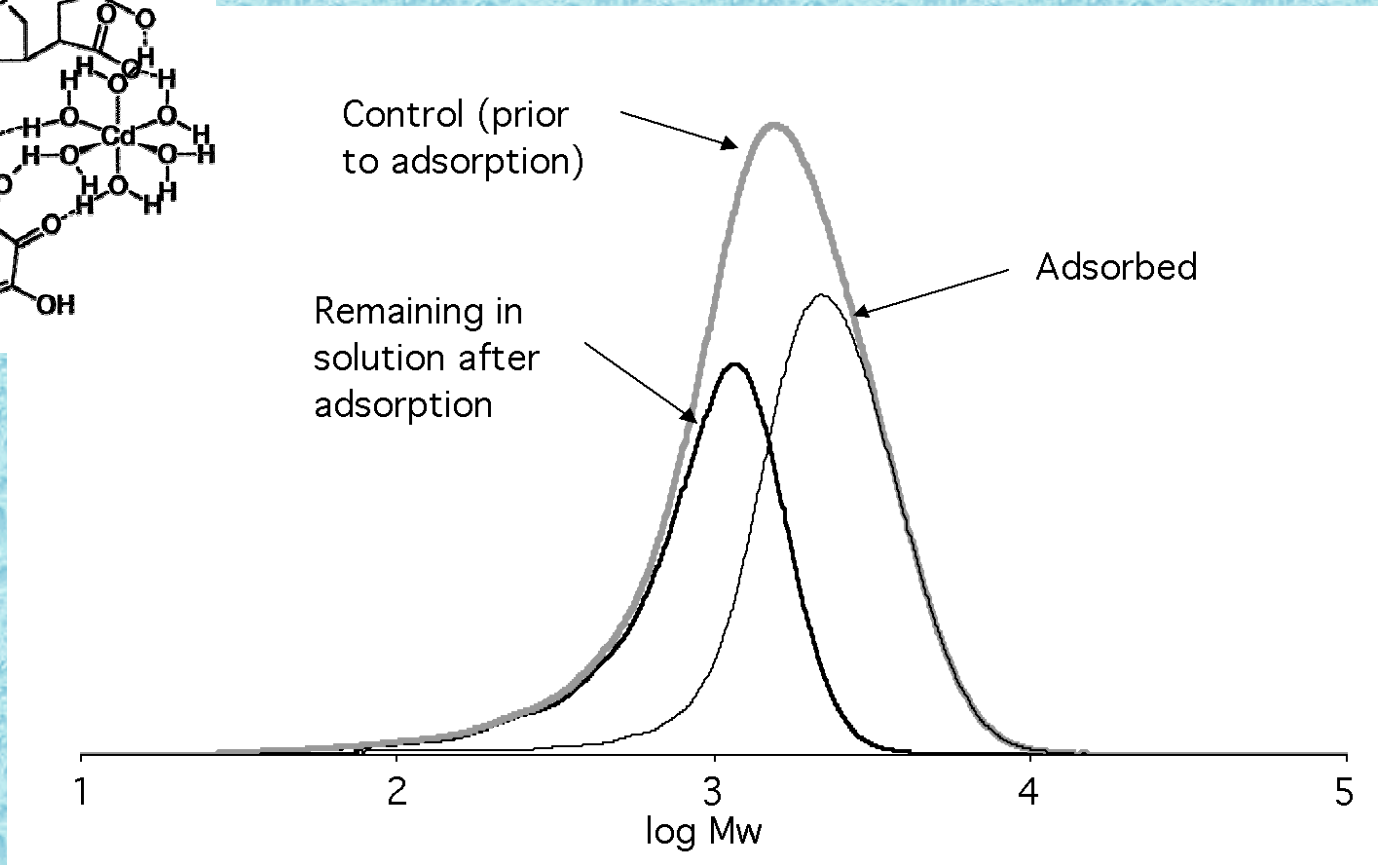
- Argonne (APS; Actinide Facility)
- Sandia (molecular dynamics modeling)
- Oak Ridge (geomicrobiology)
- DuPont Engineering Technologies

## ***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*

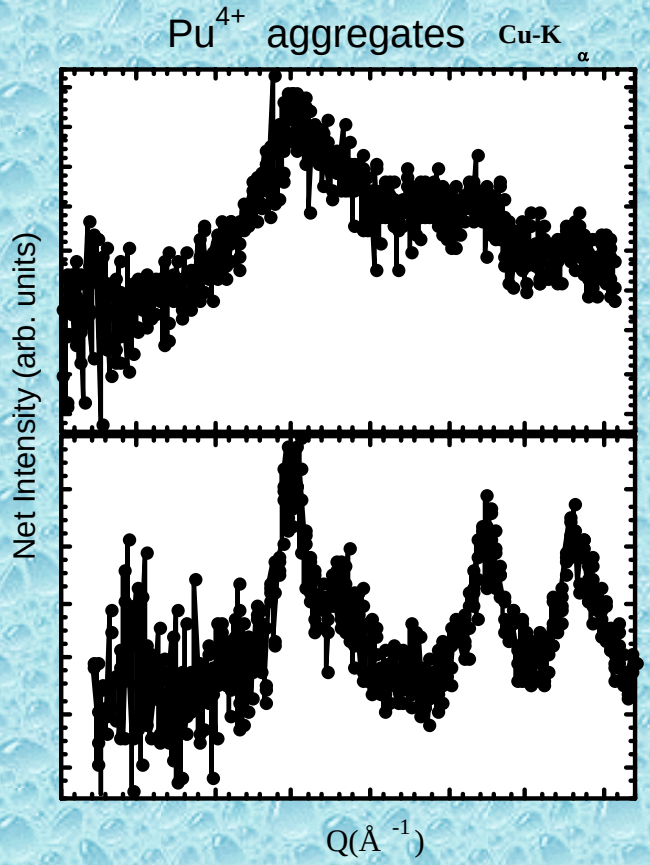


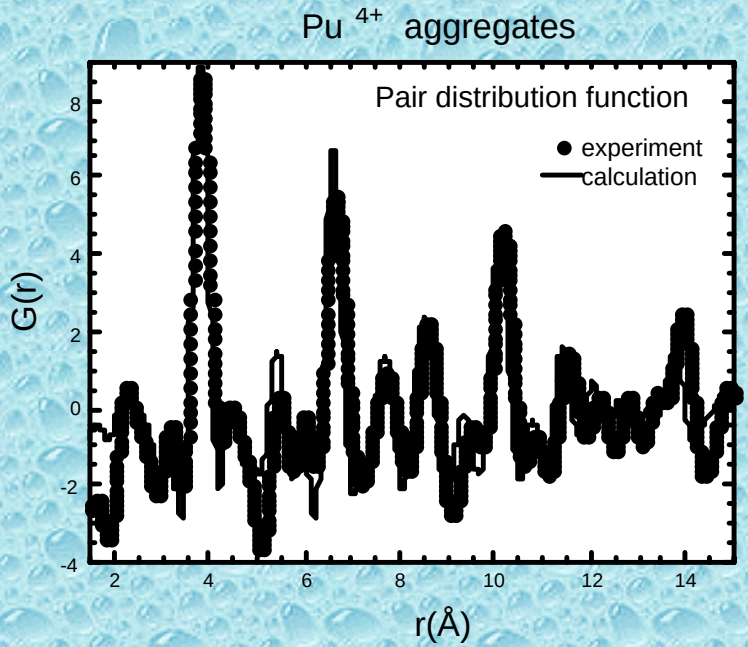

Maurice et al. (2003)

# *Nano-scale Mineral Aggregates*

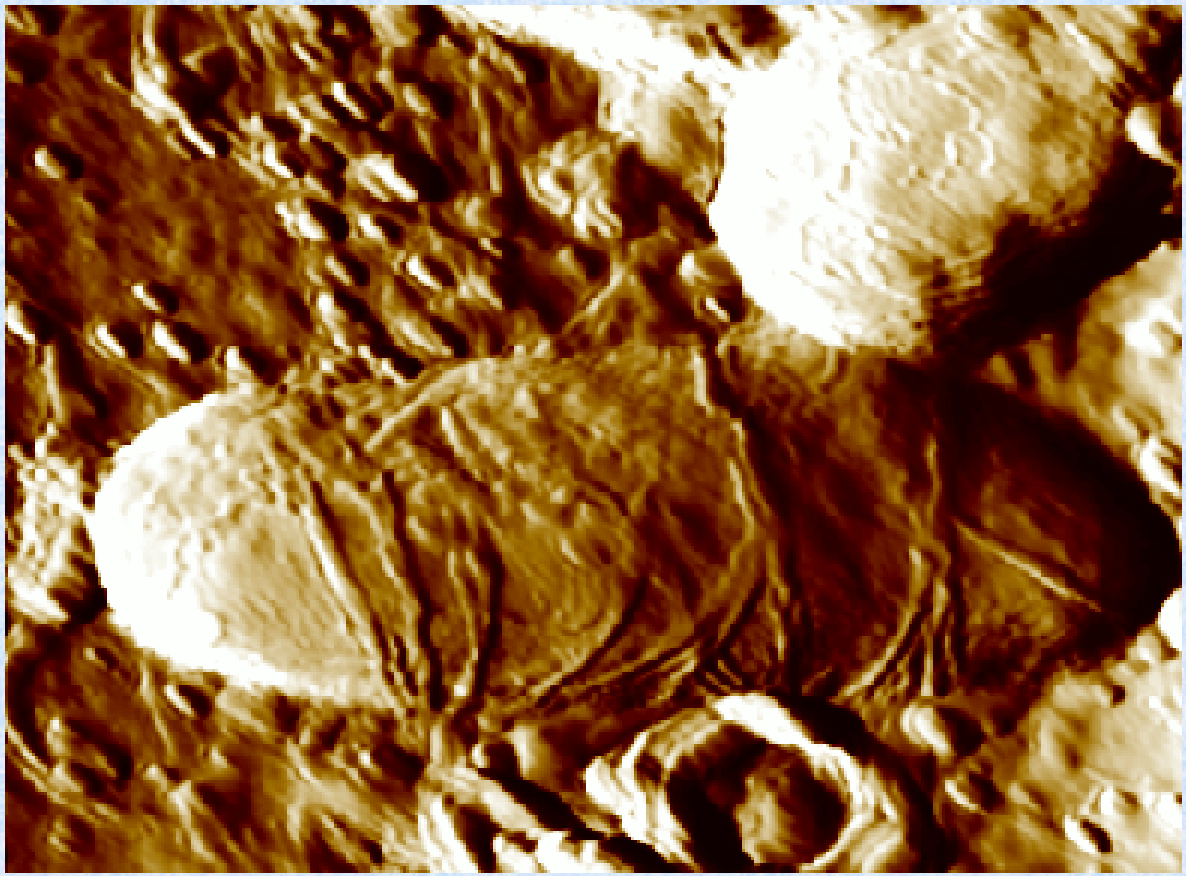
## ‘Old’ View
## Standard X-ray Diffraction

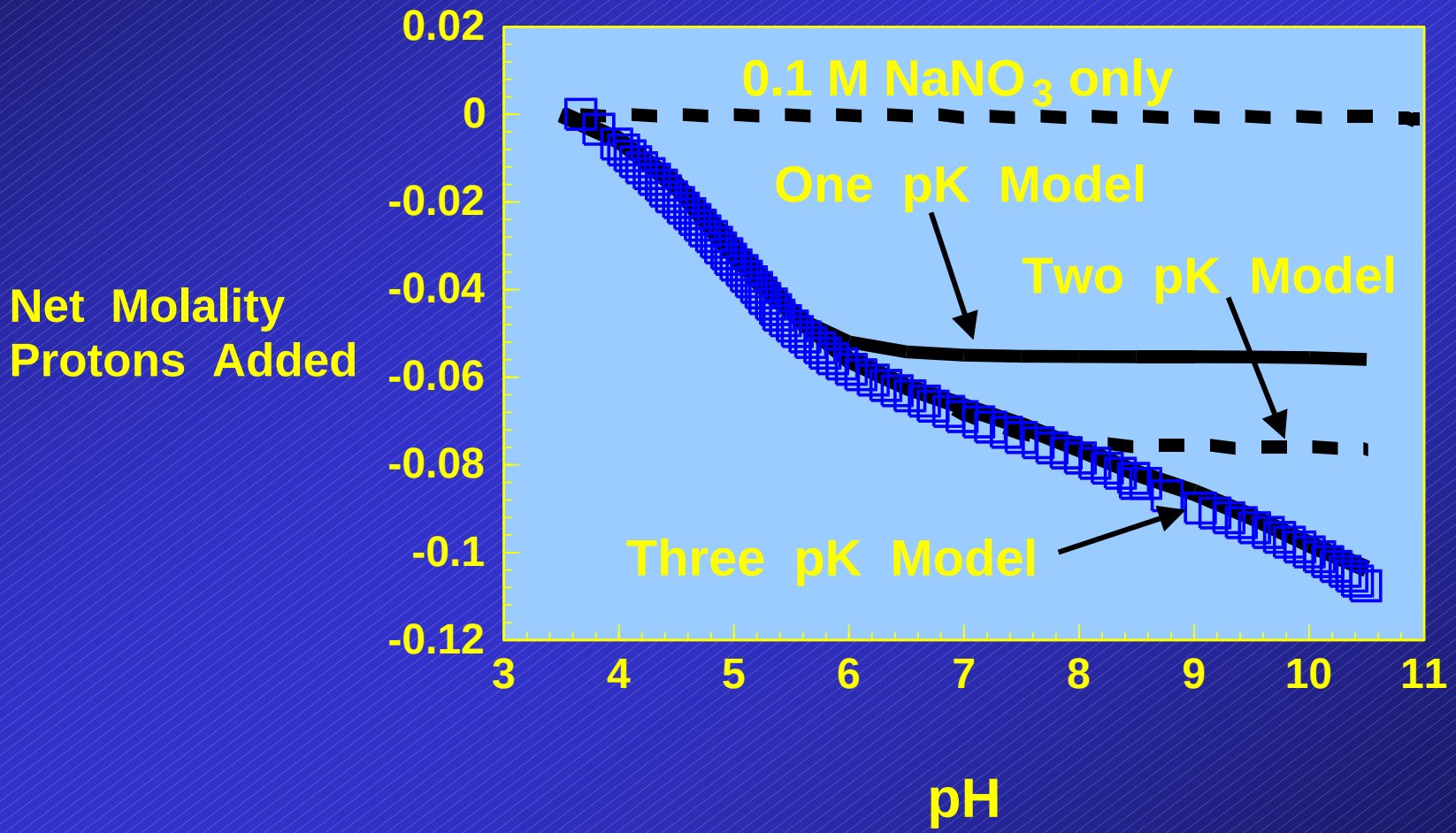



## ‘New’ View
## Advanced Photon Source
## X-ray Scattering Data



# *Bacteria-Contaminant Interactions*



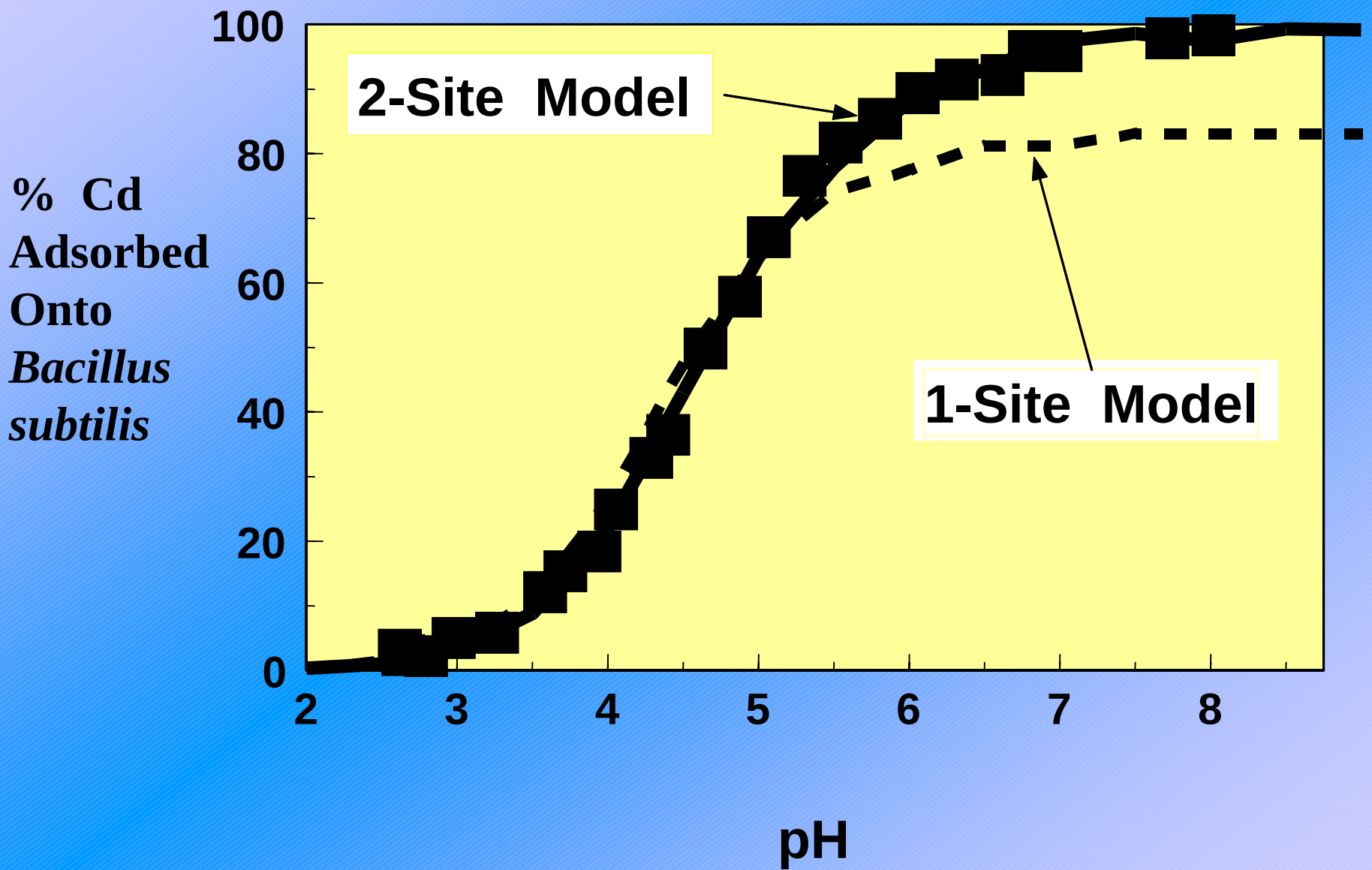

Net Molality
Protons Added
0.02
0
-0.02
-0.04
-0.06
-0.08
-0.1
-0.12
3
4
5
6
7
8
9
10
11
pH
0.1 M NaNO3 only
One pK Model
Two pK Model
Three pK Model

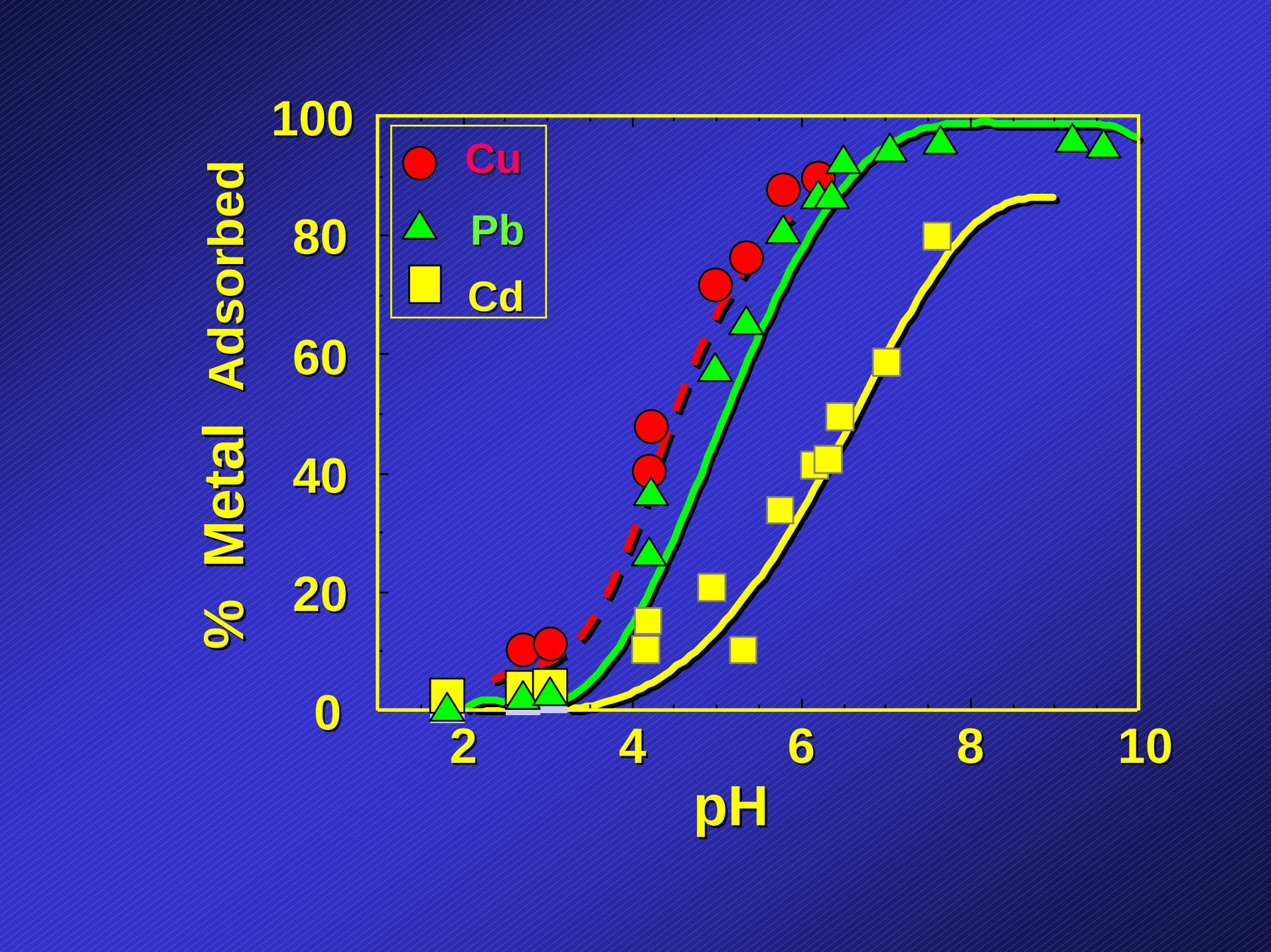
# Bacterial Cell Wall Reactions

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

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

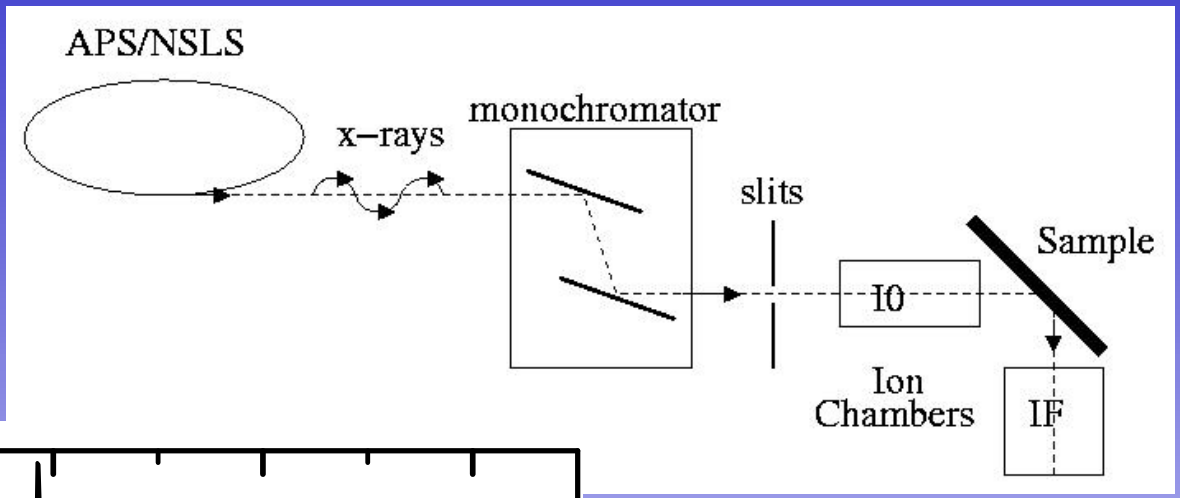
$R\text{-}OH^{o} = R\text{-}O^{-} + H^{+}$ **pKa = 9.4**

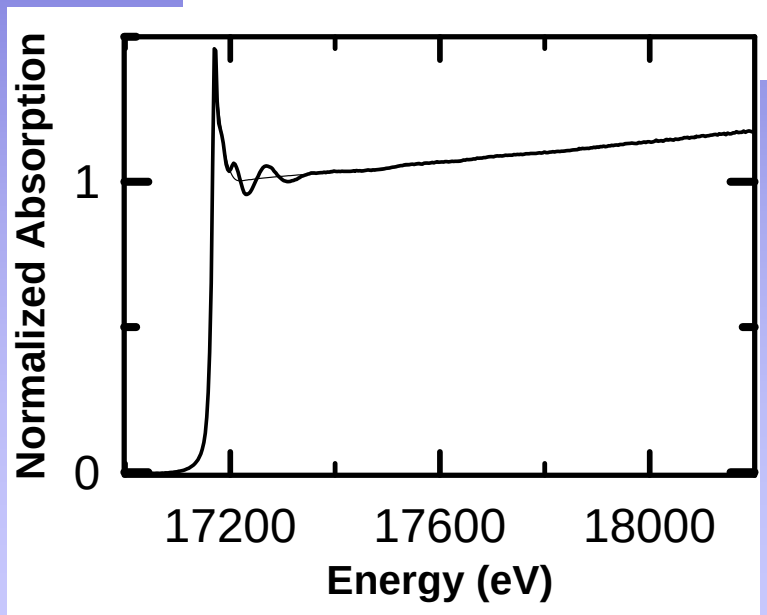

% Cd Adsorbed Onto *Bacillus subtilis*
100
80
60
40
20
0
2
3
4
5
6
7
8
pH
2-Site Model
1-Site Model


% 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



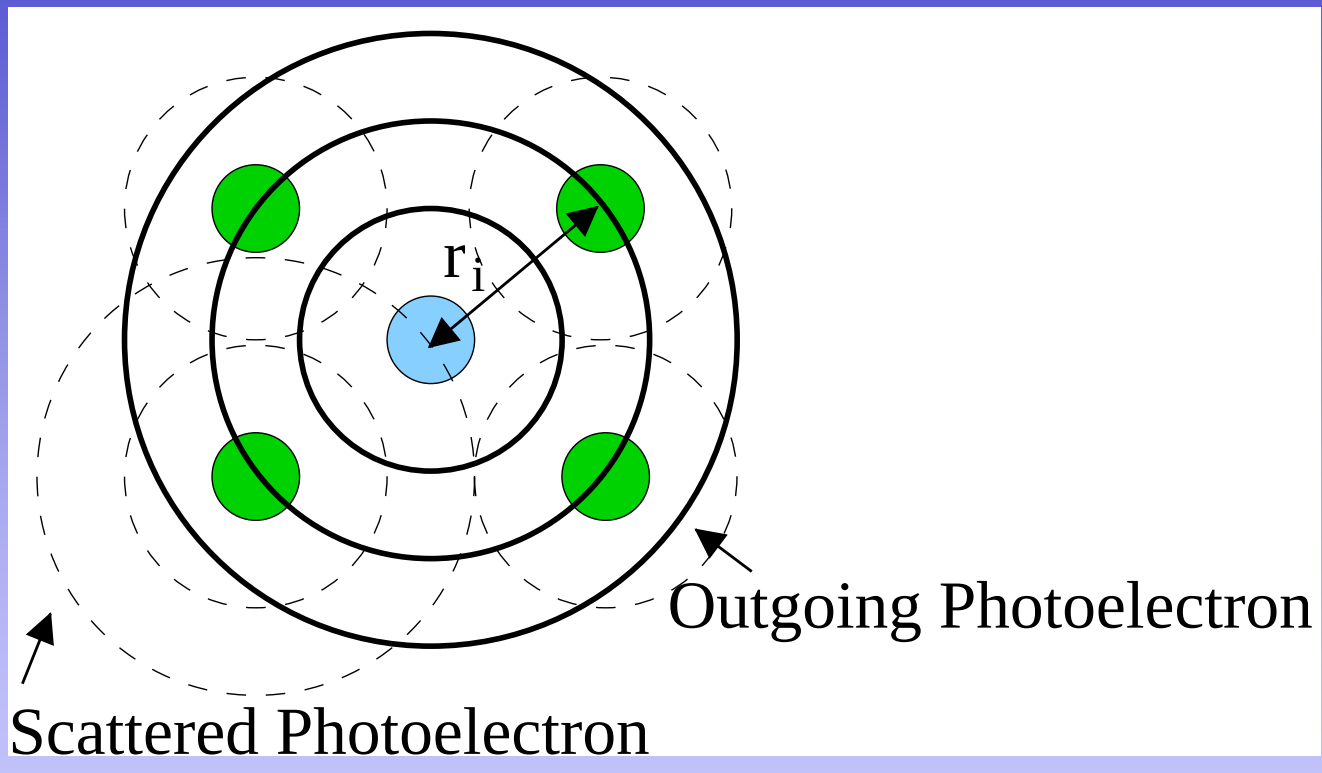

- Attenuation of x-rays

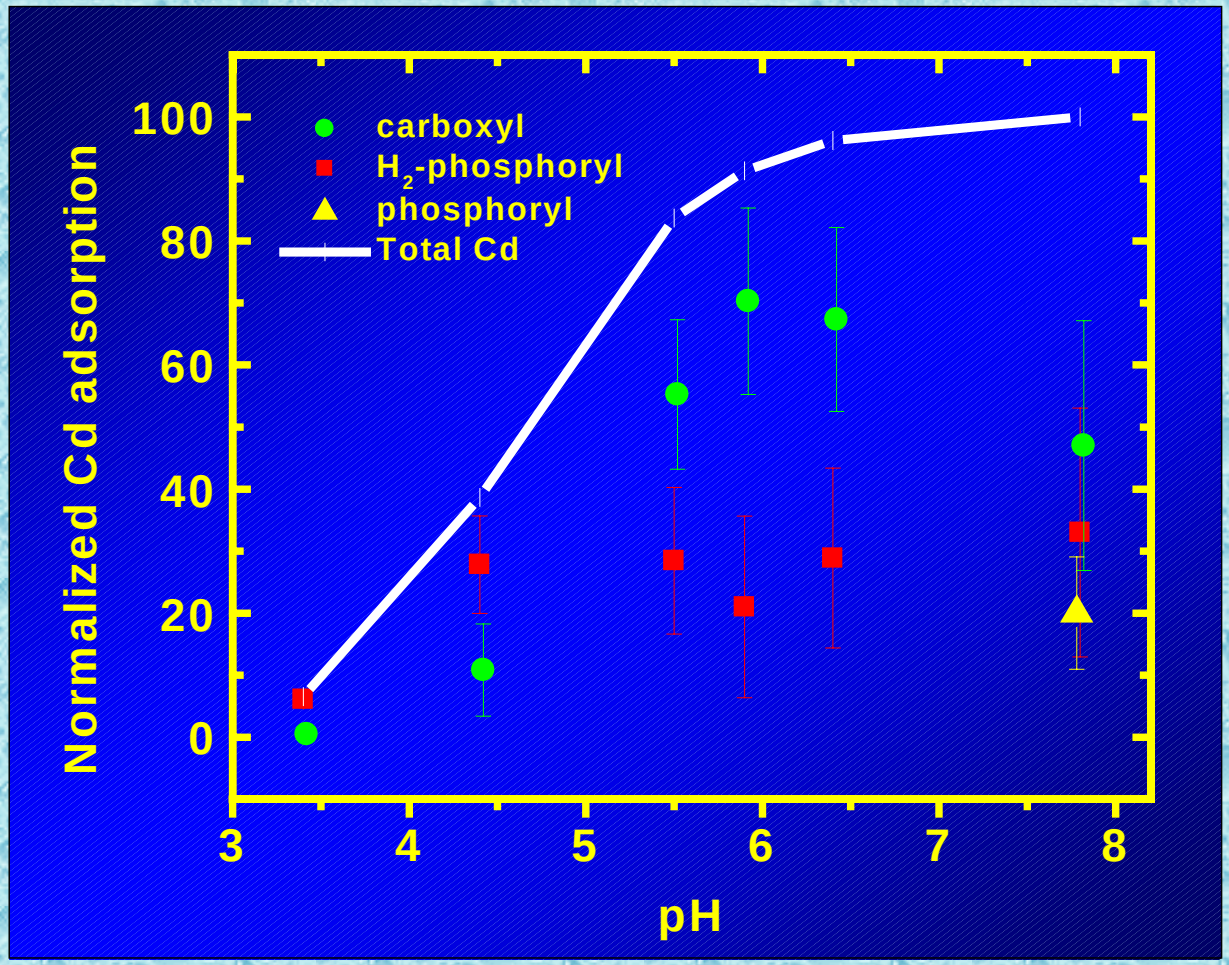
$$I_t = I_0 e^{-\mu(E)\cdot x}$$

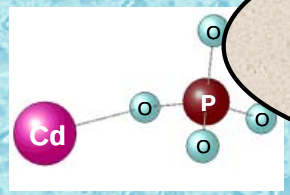
- Absorption coefficient

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

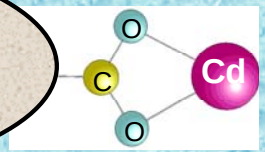
# X-ray-Absorption Fine Structure



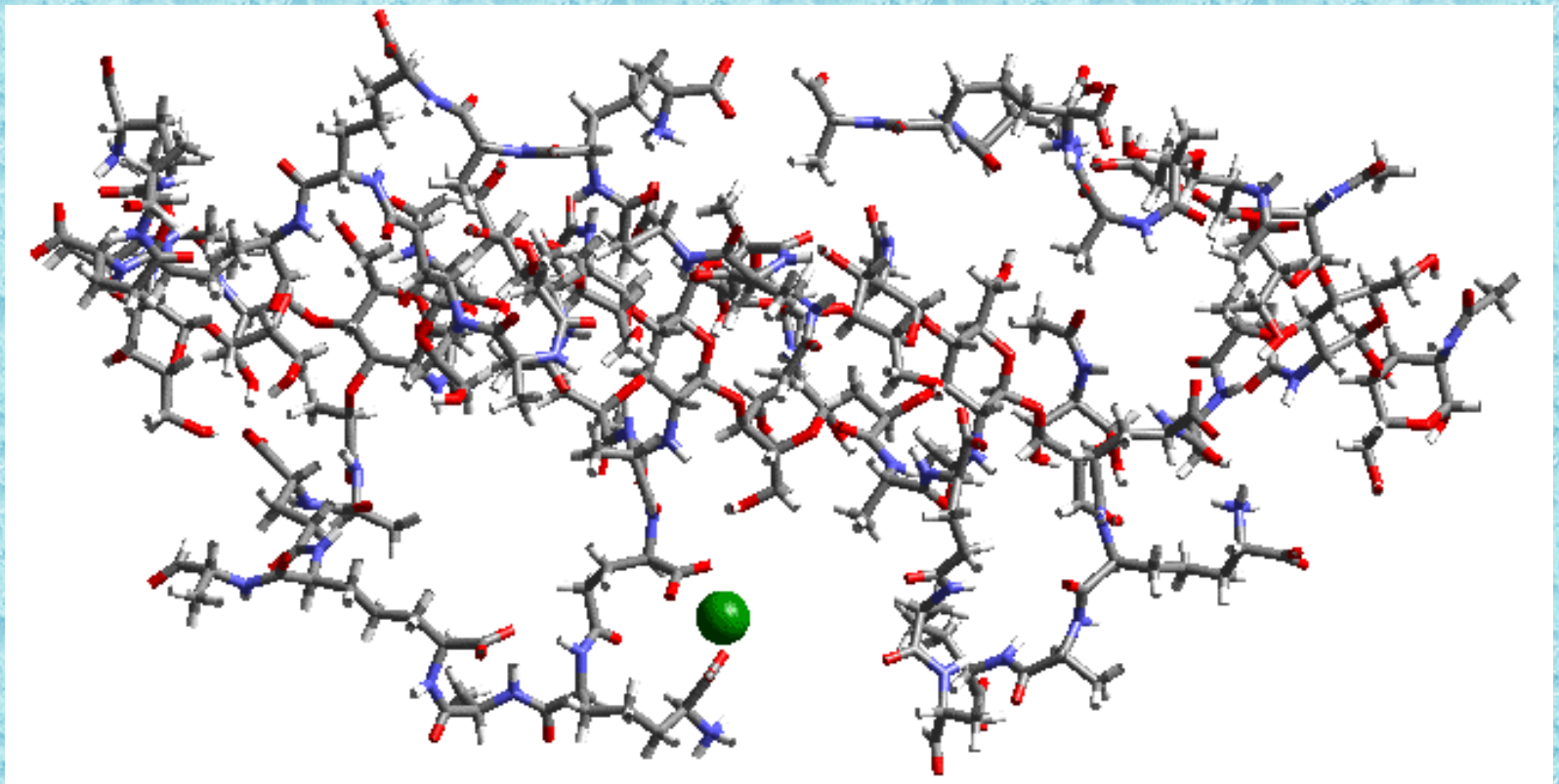


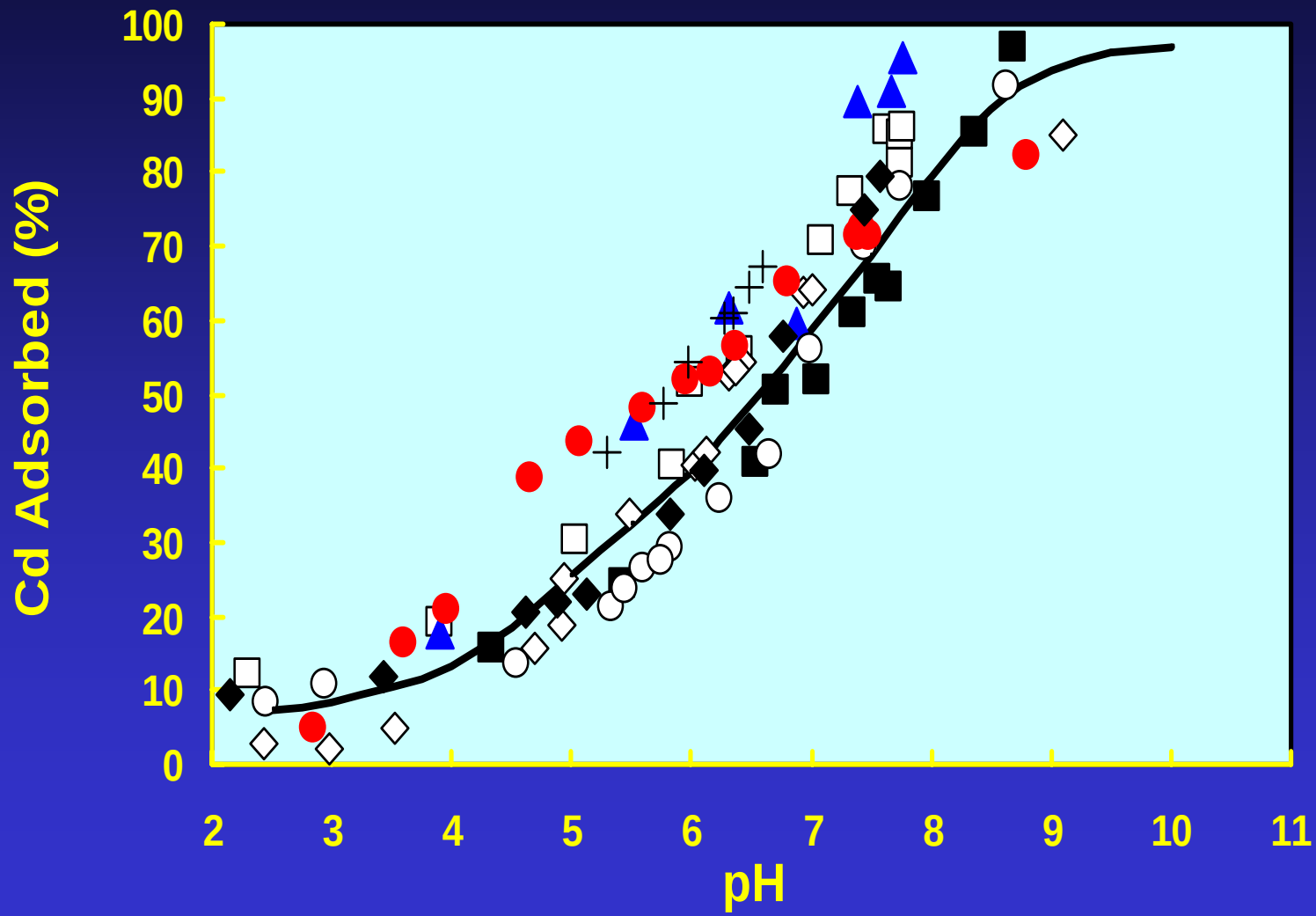

**Bacterial surface**
**5 μm x 1 μm, 140 $m^2$ /g cell**



# 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.**