

<http://www.cosmic.mse.iastate.edu>

## Informatics for Nanomaterials Discovery and Design

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Iowa State University, Ames IA



Homeland  
Security

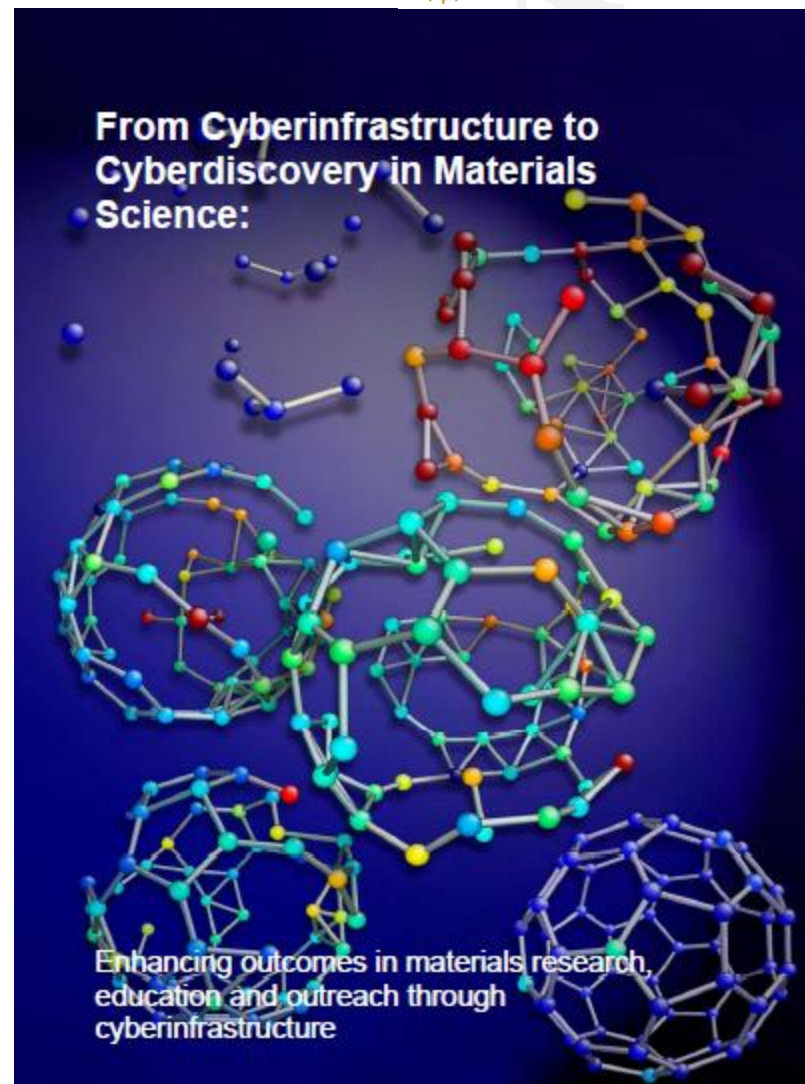


Nanotoxicology vs. Nano drug delivery

Nano – sequestration of Toxic Elements

Nanoinformatics & Cyberinfrastructure

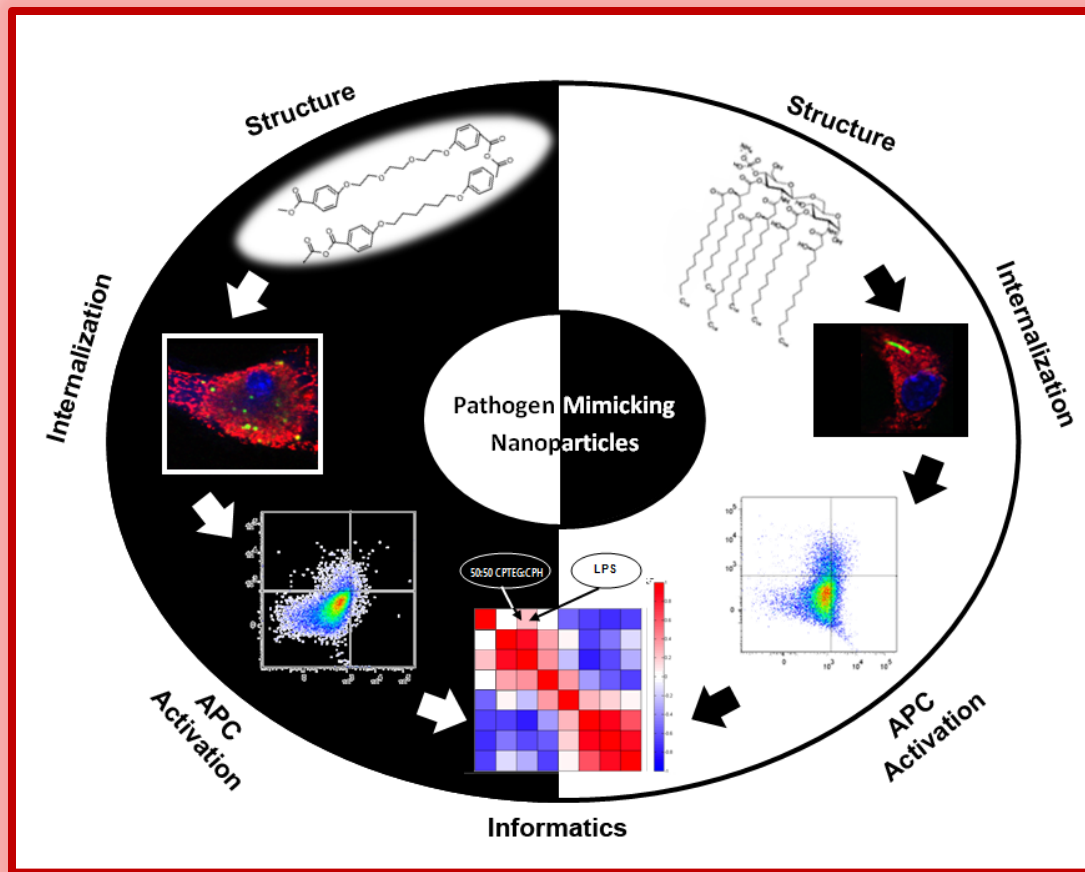
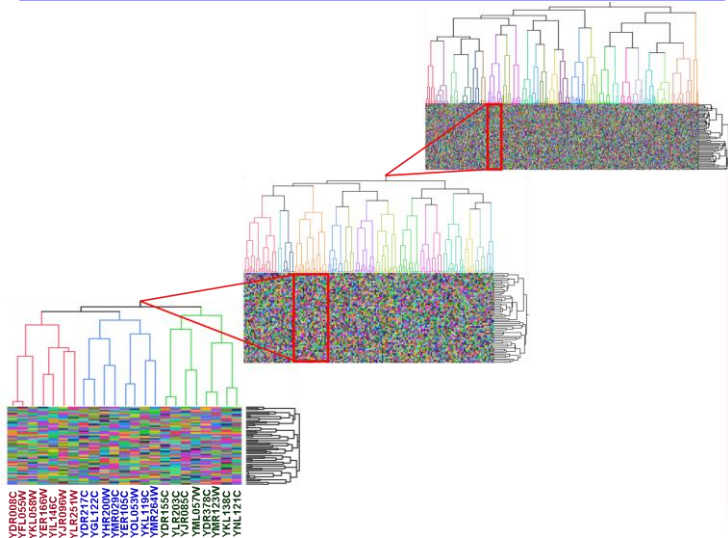
Nanoinformatics & Cyberinfrastructure



S. Billinge, K. Rajan and S. Sinnott (2006)

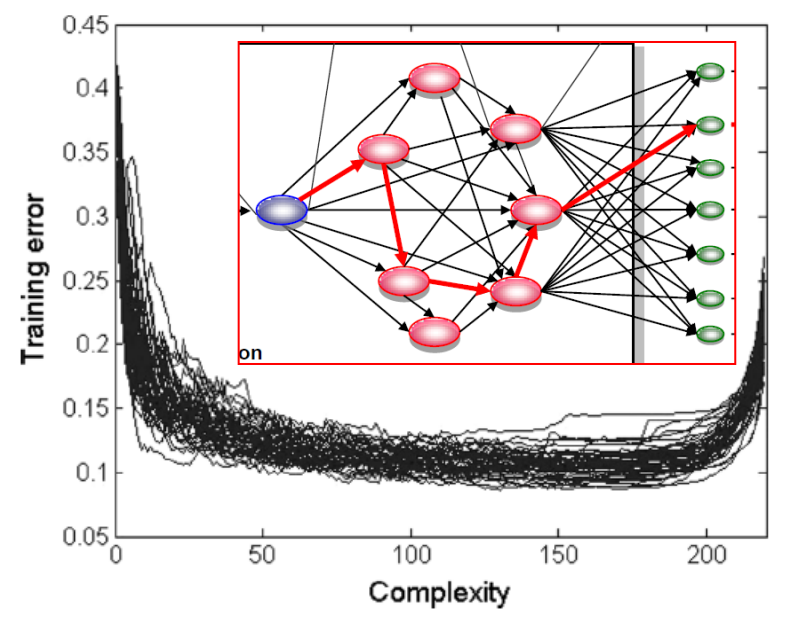
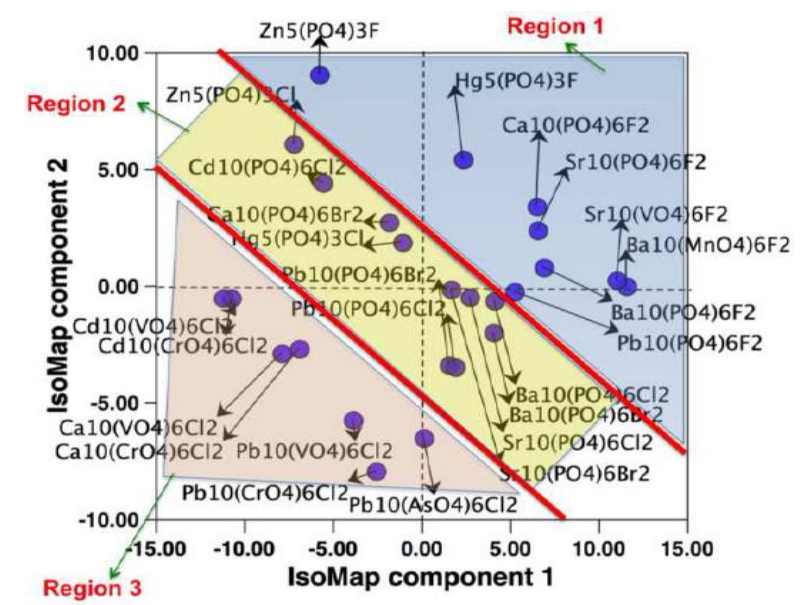
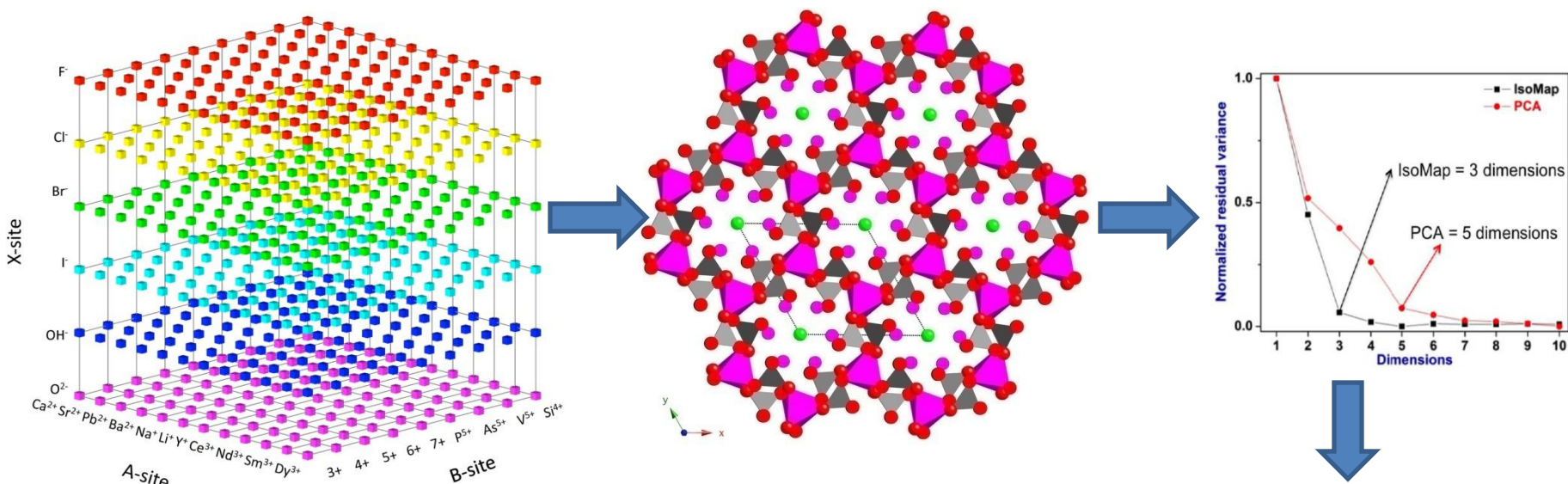
- Designer Materials for Designer Drugs
- Engineered Nanoparticles: Pathogen Mimicking Nanoparticles

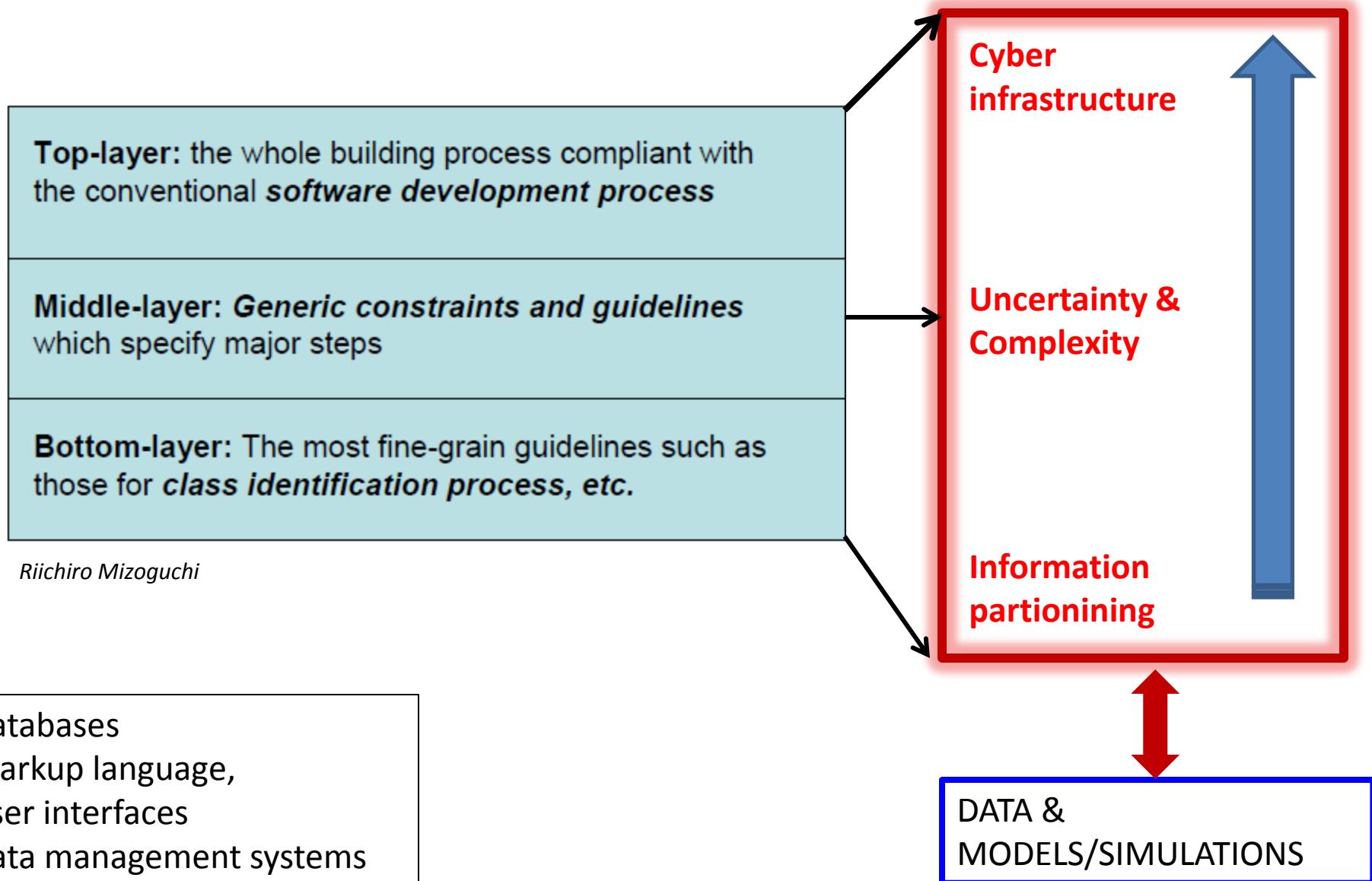
- Molecular structure data
- Descriptor data
- Framework for linking descriptors to materials properties – graph theory





# Nano – sequestration of Toxic Elements





Riichiro Mizoguchi

databases  
markup language,  
user interfaces  
data management systems

ThinkSpace - Mozilla Firefox  
File Edit View History Bookmarks Tools Help  
https://portal.iastate.edu/thinkspace/gwt/UserSpace.html?pid=1255  
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my Space 3D Atom Probe  
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Introduction Data Informatics Result PC Result Physics Case Study Conclusion Interpretation Interpretation  
Search sequence  
High Light yield scintillators

- Density < 4.01 and
- Stoke >2488 and
- Valence electron factor >4.9 and
- Size factor is <1.28 and
- Electrochemical factor > 1.903

Density  
Atomic number  
Photoabsorption coefficient  
Attenuation length  
Field depression  
Stokes shift  
Valence electron factor  
Size factor  
Electrochemical factor  
1 of 1  
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