

# Scientific Opportunities in Computing for Energy Storage

*James W Davenport*

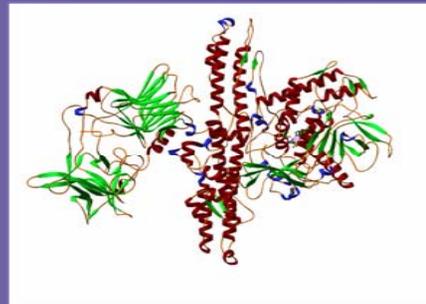
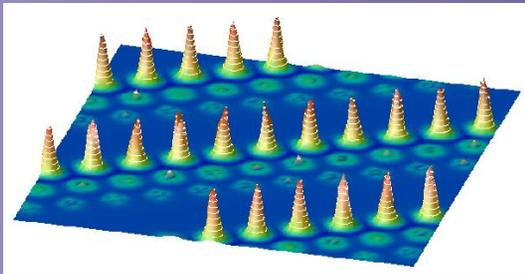
*Computational Science Center*

*Center for Functional NanoMaterials*

*Maui, January 11, 2008*

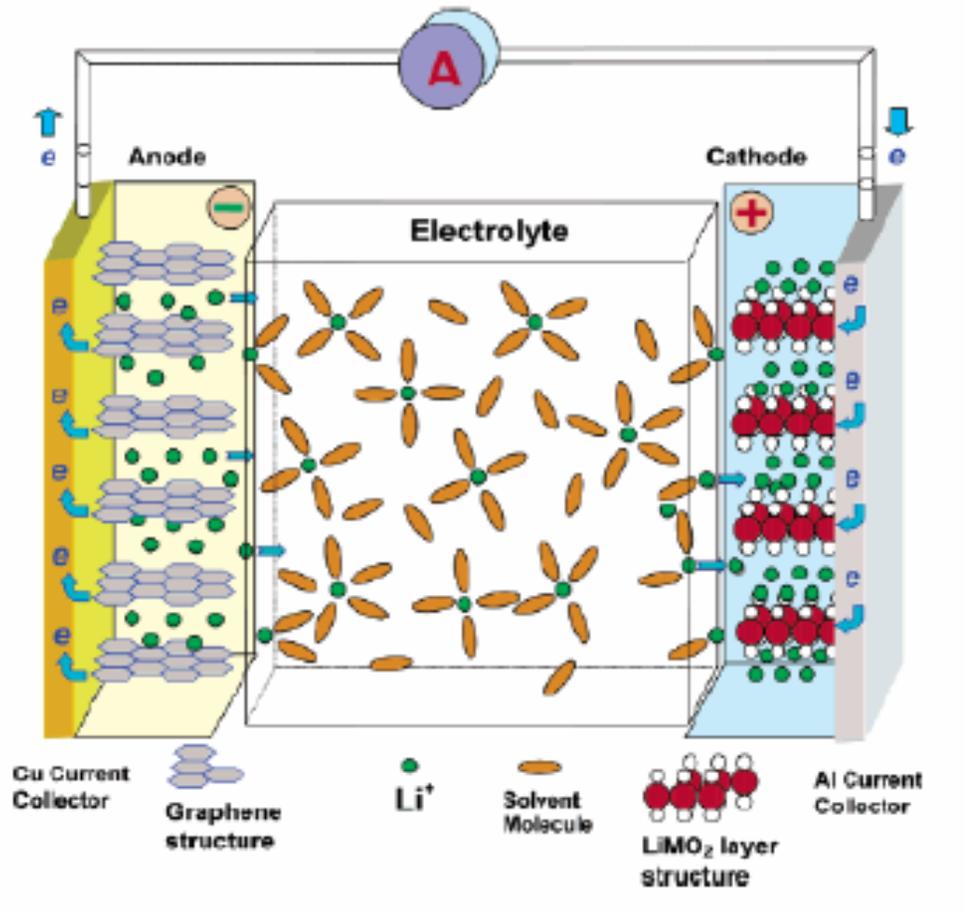


SIXTY YEARS  
OF DISCOVERY  
1947-2007



**BROOKHAVEN**  
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# What is a Battery?



Basic Research Needs for Electrical Energy Storage

# What is a Battery?

- Complex Systems
- Multi-Phase
- Chemically Reacting - Ion Motion
- Mixed Materials - Organic/Inorganic/Metal/Oxide
- Multi-Scale
  - Atomic - Macroscopic Dimensions
  - Multiple Time Scales
- Entropy, Free Energy, ala hydrophobicity
- Properties Shared by Biological Cells

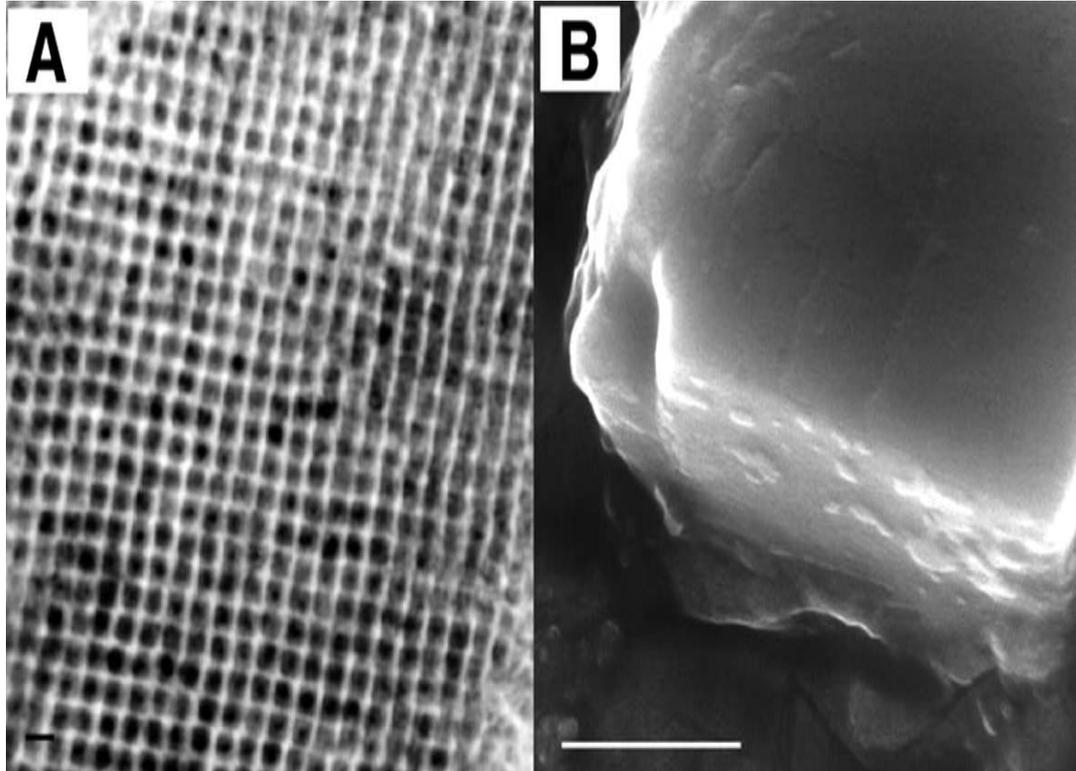
# BES / BRN Report

- Thermodynamic Properties of NanoScale Systems
- Liquid - Solid Interface
- Chemical Reactions
- Intercalation
- Ionic Conductivity / Ion Channels
- Surface Structure at NanoScale
- Adsorption

# Hierarchy of Standard Tools

- Quantum Mechanical
  - Ab-Initio, DFT
- Car-Parrinello or First Principles MD
- Force Field MD
  - AMBER, CHARMM
- Heisenberg Magnets
- Nano-particle – Nano-particle
- Continuum
  - Elasticity, Micromagnetics

# Iron NanoCubes

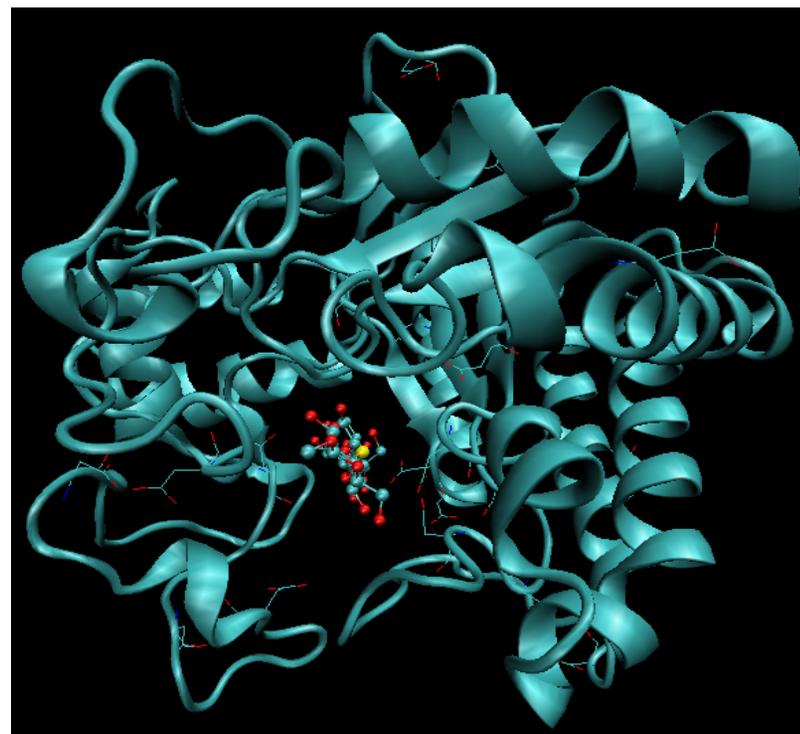


Assembly of iron nanocubes  $7 \times 7 \times 7 \text{ nm}^3$

Dumestre et. al. Science 303, 821 (2004)

# System - Cel6A

- Crystal structure (1KQ2)
- Acid proposed (Asp122)
- **Base uncertain** (*pKa shifts*)
- Simulations details:
  - GROMACS 3.3.1 (ffG53a6)
  - solvated system  $\approx$  40K atoms
  - 10  $\lambda$  windows charging FE
  - 20  $\lambda$  windows  $\Delta$ LJ FE
  - temp 300K, 2 fs timestep
  - reaction field

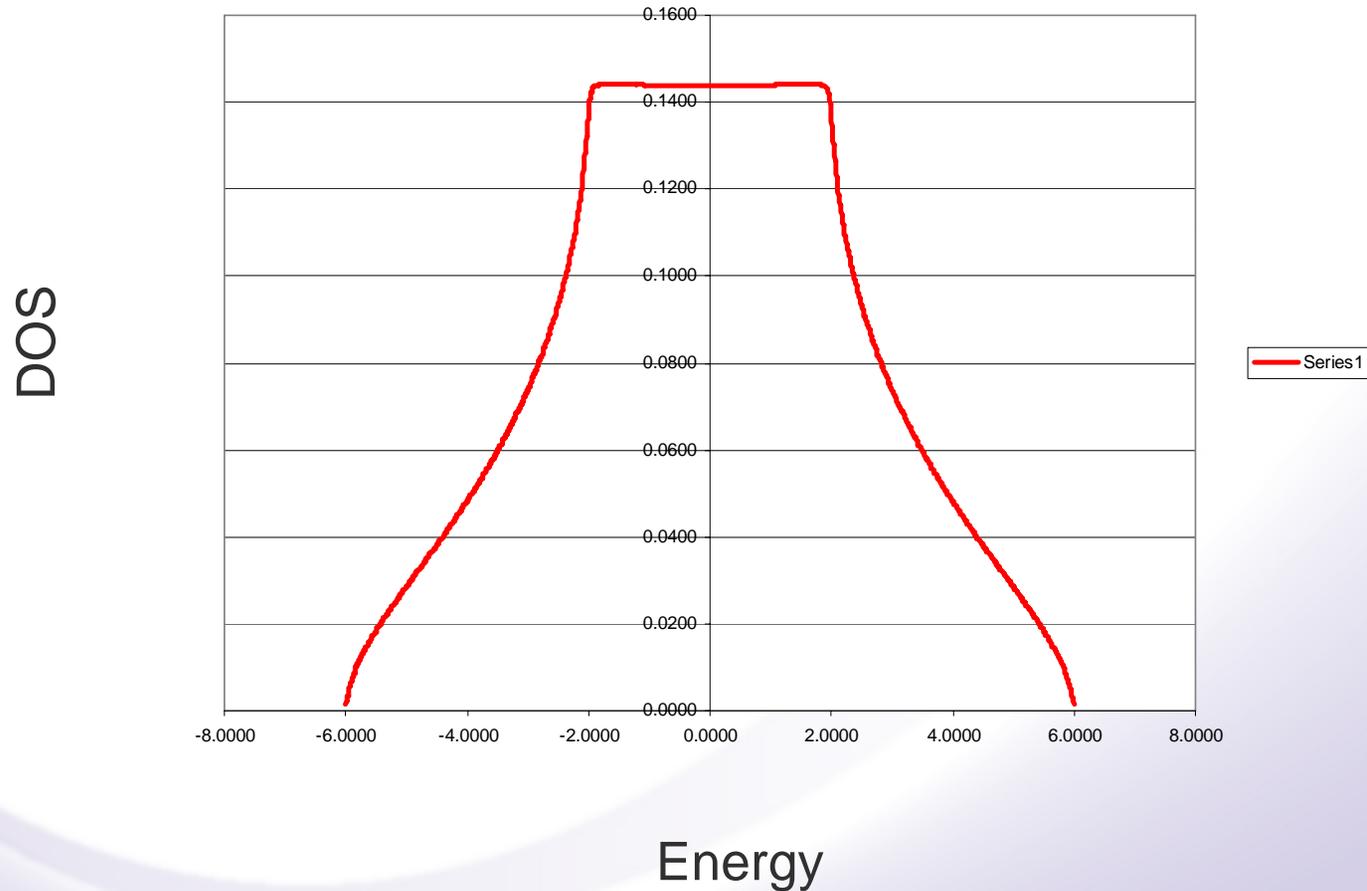


# Quantum Solutions

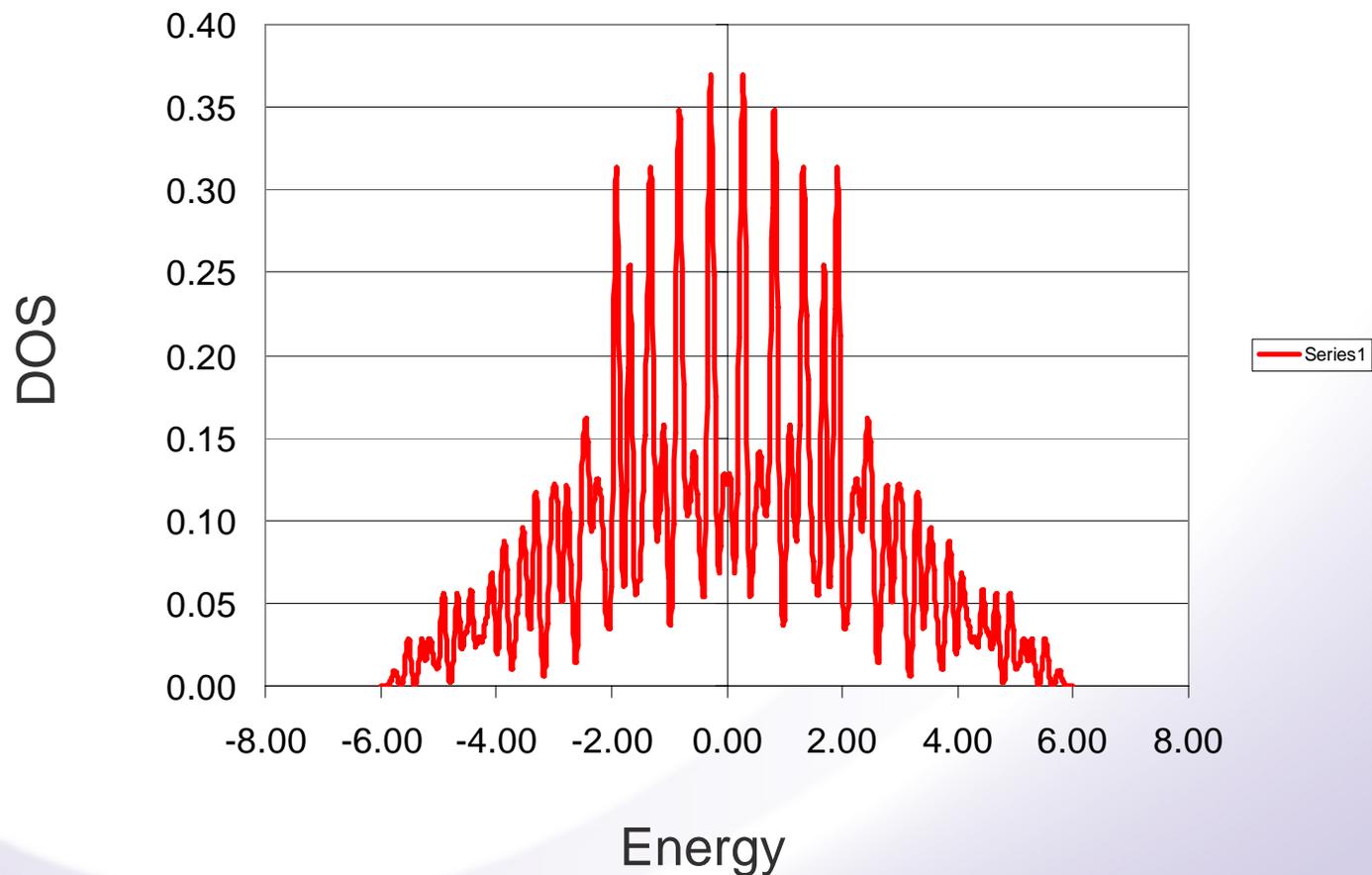
- Schrodinger Equation
  - 1 particle: PDE in 3 variables
  - N particles: PDE in 3N variables
- Multiparticle  $\sim e^N$ 
  - using basis with one orbital / atom
  - $\sim 20$  sites by exact diagonalization
  - $\sim 1000$  sites by quantum Monte Carlo
  - very limited basis set
- Hartree-Fock
  - single determinant  $\sim N^4$
- Density Functional Theory
  - approximate many body solution from *single particle* Schrodinger equation
  - $\sim N^3$

# Density of States

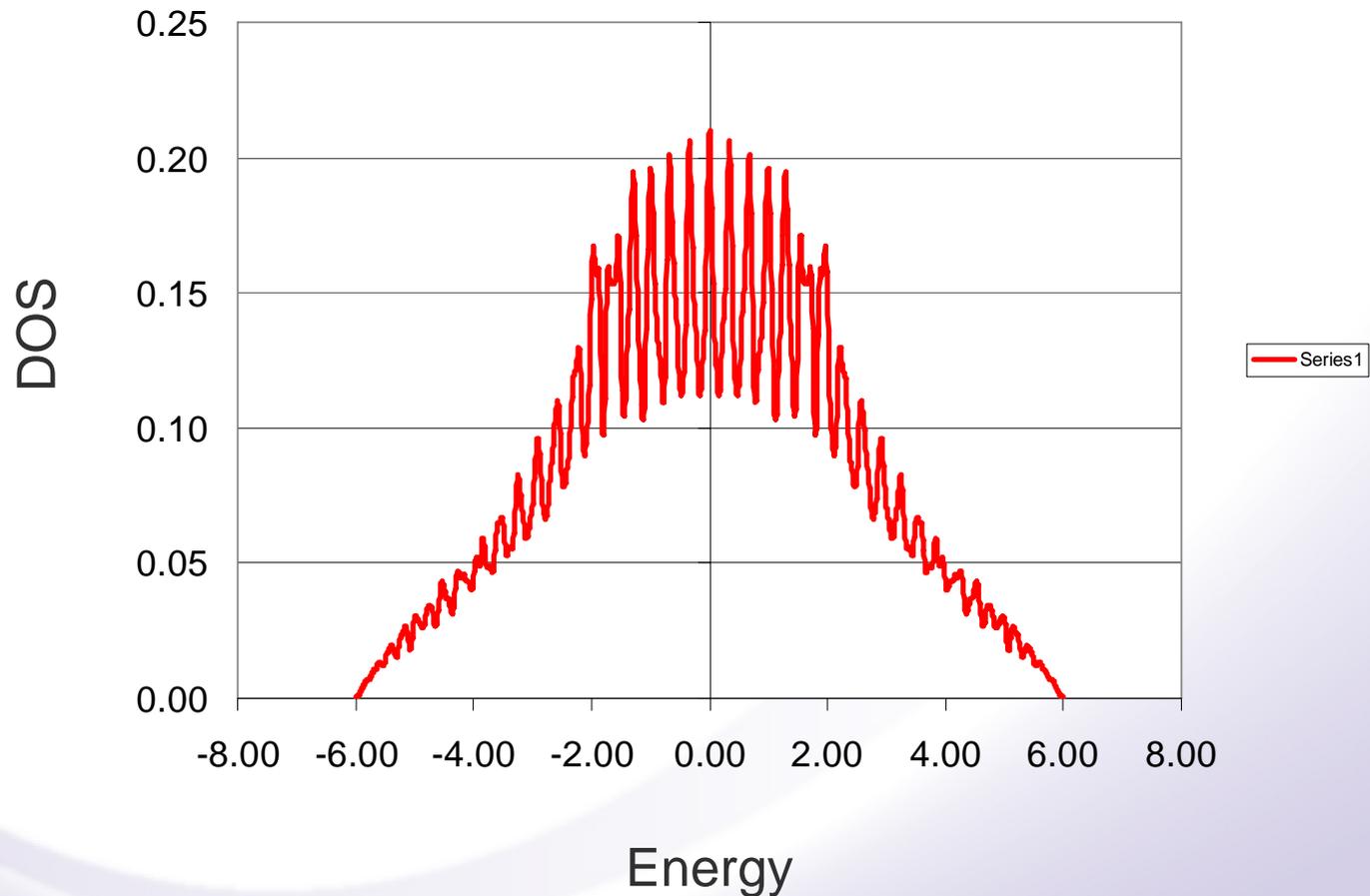
## 1,000,000 Atoms (100x100x100)



# Density of States - 10000 Atoms



# Cluster Density of States 4913 Atoms (17x17x17)



# Molecular Dynamics

- Newton's equations,  $F = M a$
- Force Field
  - Semiempirical
  - Long Range
    - Coulomb, Lennard-Jones
  - Short range
    - Bond stretching, bending
  - CHARM, AMBER

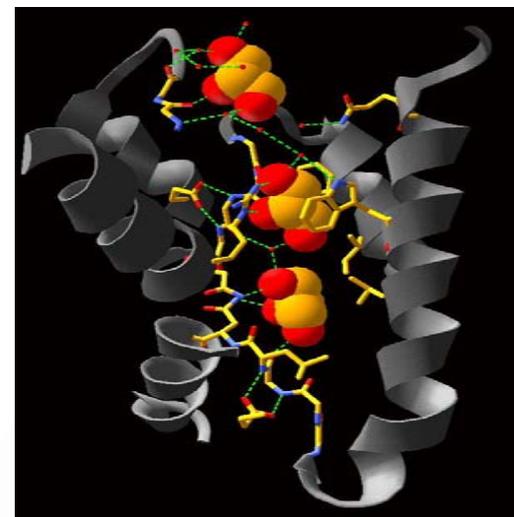
$$E_{\text{total}} = \sum_{\text{bonds}} K_r (r - r_{\text{eq}})^2 + \sum_{\text{angles}} K_\theta (\theta - \theta_{\text{eq}})^2 + \sum_{\text{dihedrals}} \frac{V_n}{2} [1 + \cos(n\phi - \gamma)] + \sum_{i < j} \left[ \frac{A_{ij}}{R_{ij}^{12}} - \frac{B_{ij}}{R_{ij}^6} + \frac{q_i q_j}{\epsilon R_{ij}} \right]$$

# Molecular Dynamics

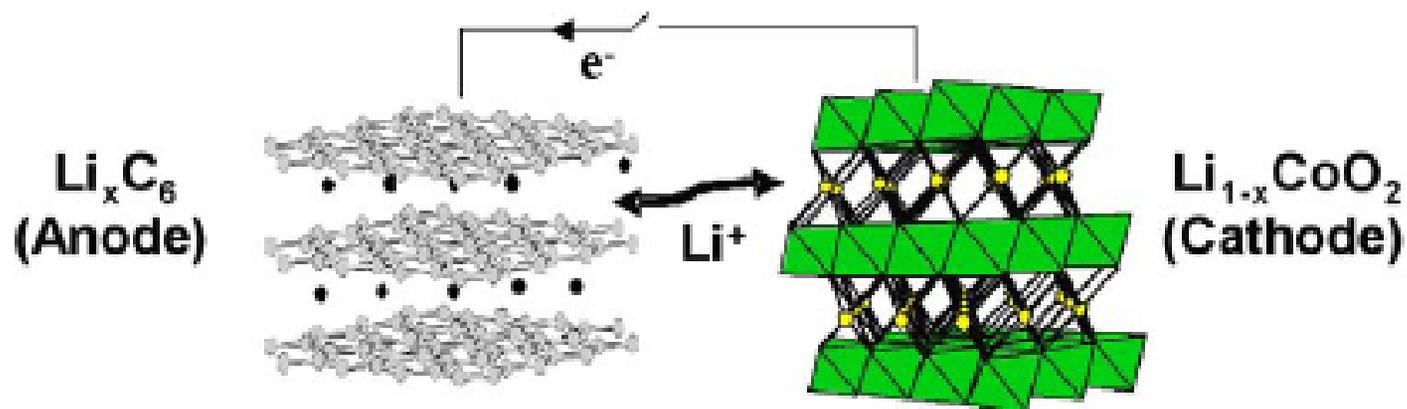
- Time step,  $\Delta t \sim 10^{-15}$  seconds
- Microsecond =  $10^{-6}$  seconds
- $10^9$  time steps
- On Blue Gene/L
  - 100,000 particles / 10,000 processors
  - 10 particles / processor
  - communication less than computation

# Molecular Dynamics Example

- Aquaporin - 106,189 atoms
- MD simulation
- Tajkhorshid et. al.
  - Science (2002)
  - 10 nanoseconds simulated time
- Structure by Dax Fu et. al.
- Blue Gene/L
  - 1 – 10 microsec simulated time
  - few weeks wall clock
  - Int J High Performance Comp App, **18**, 183 (2004)



# Lithium Ion Cell

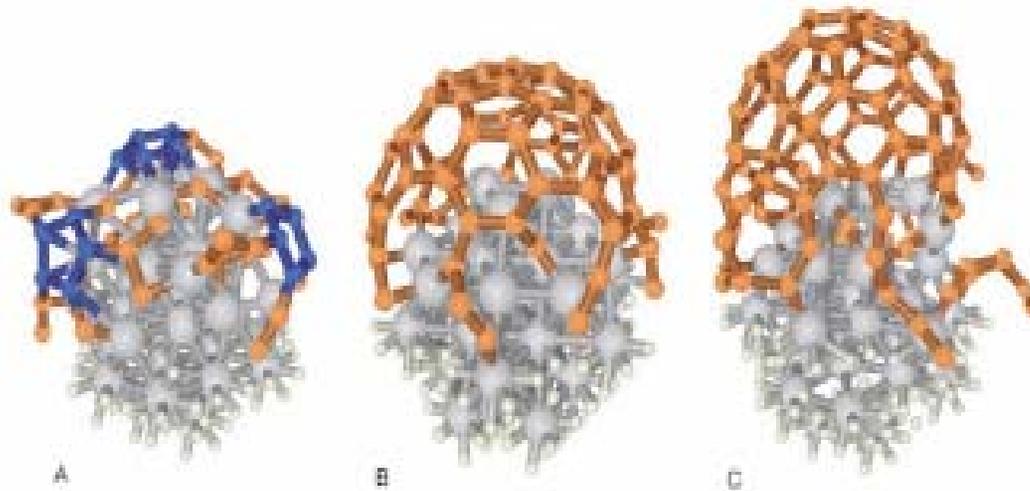


Basic Research Needs for Electrical Energy Storage

# *Ab Initio* Study of Growth of Carbon NanoTubes on Iron

Combined quantum mechanics and MD

Forces computed on the fly from Hellmann-Feynman



Raty, Gygi, & Galli, Phys. Rev. Lett. (2005)

# Research Needs

- Span length and time scales
- Planning for petaflop/s
- Interoperative codes
- Standards for data sharing
- Community effort
- Plan for data storage and retrieval
  - data repositories
  - data mining

# New York Blue



# NewYorkBlue

- 100 teraflops Blue Gene/L
  - Gigabyte memory / Node
  - 2 x other BG/L machines
- 28 teraflops Blue Gene/P
- NWChem
  - small Pd and Au clusters
- CPMD
- QCD, WRF, AMBER, NAMD.....

# Summary: Opportunities in Energy Storage

- Golden Opportunity
- Problems are at the edge of where these fields are going anyway
- Very attainable
- Couple to data repositories, combine with experimental probes (like cryo-em).