Breakout Report on Correlated Materials

Identification of Grand Challenges
Breakout - correlated materials

- Chairs: Littlewood (Argonne), Parkin (IBM)
- Speakers: Terris (HGST), Kotliar (Rutgers)
Correlated materials

- Not just emergent properties (magnetism, superconductivity)
- Battery electrodes (ideal Li-ion cathode is a Mott insulator)
- (Electro-) chemistry at interfaces
- Combustion chemistry
Engineering driven modeling and characterization tools
The consequence of understanding is prediction: Moore’s Law for Si vs. current strategy for Li-ion batteries

- **Unk-HV-HC / Li metal**
  - Safe and reversible cycling of Li metal
  - Market entry >2021

- **Unk-HV-HC / Gr-Si**
  - Discovery of high voltage electrolyte >4.8 V
  - Discovery of reversible unknown high-voltage high-capacity cathode: 250 mAh/g @ 4.8 V
  - Market entry > 2019

- **Li₂MXO₄ / Gr-Si**
  - Discovery of path to reversible multi-electron cathode material with 4V cell voltage
  - Market entry > 2017

- **LMR-NMC / Gr-Si**
  - Stabilization of silicon
  - Market entry > 2015

- **LMR-NMC / Gr**
  - Stabilization of LMR-NMC
  - Market entry > 2013

- **LMO / Gr**
Computational Chemistry and Materials Science: designing what you make

- Prediction of new materials and structures on the atomic scale, including interfaces, growth and defects
- Accurate intermolecular potentials to model structure and dynamics on nanoscale
- Excited state calculations for electron transfer and photon-mediated transitions
- Semi-classical models of electrical and particle transport on mesoscale
- Effective theories of inhomogeneous media: elastic, fluid and electrical transport

- Each box requires new investment in methods, theory and computation
- Joining up the boxes is as important as the investment in any single piece
- We must curate both data and software
- Design choices driven by application target

Demands a collective corporate effort linking computation, methods, software, and data guided by an engineering goal
Better superconductors - design of vortex pinning for large current applications

\[ F_{GL} = \frac{1}{2} \int d^d x \left\{ \beta \left( \frac{\alpha}{\beta} + |\psi|^2 \right)^2 + \frac{\hbar^2}{m} \left| \left( i \nabla - \frac{2\pi}{\phi_0} A \right) \psi \right|^2 + \frac{1}{4\pi} (\nabla \times A - H)^2 \right\} \]

Time-dependent Ginzburg-Landau eqn.

Equations well understood: but contain long range forces, disjoint length scales, and need long times

BES-SCIDAC – Andreas Glatz, Argonne
Theory and experiment meet around “big data”
Spin fluctuations in a quantum paramagnet (Collin Broholm)

Large N expansion: Nearest Neighbor Interactions only (Chalker and Conlon)

$J_2 = 0.2$, $J_1, J_{3a} = 0.2$, $J_1, J_{3b} = 0.01$ (Chalker and Conlon)

Mourigal, McQueen, Koohpayeh et al.
Building multiscale models via “genomics”
Materials by design: genomics?

Genomics must be grounded in theory: the human genome initiative depends fundamentally on the “central dogma” of DNA coding. This is both the fundamental theory of biology and an algorithm.

Materials genomics derives its validity from the Schrodinger equation – but this is not (yet) an instruction set.
Supervised learning: Gaussian Approximation
Potentials trained on DFT (Gabor Csanyi)

Theoretical limit for given cutoff: RMS of long range forces

Diamond (1000 K)

Energy error < 1 meV (0.02 kcal/mol) / atom
Engineering pull
Materials/product engineers need to be able to __A______, which materials scientists could enable by ___B______.

A
- Make textured materials
- Control materials growth
- Engineer vortex pinning in superconductors
- produce layered combination of materials with large resistive response, controllable anisotropy of magnetic layers
- Defect control in oxides
- Sub 10-nm device fabrication
- Nano 3D printer

B
- Multiscale modeling
- In operando theory
- Connect ab initio to GLAG theory
- spin dependent transport simulations, rational design of magnetic anisotropy
- appropriate models/theory of defects and interfaces
- Theory of etching
- Develop advanced ALD
Science push: Materials discovery
If we could do __A__, it would make possible _B___ new pathways of materials discovery.

A
- Develop “good enough/robust” models for structure, defects excitations, transport across scales
- Predictive capabilities for correlated (solid/solid or solid/liquid) interfaces
- Rapidly survey strongly correlated materials
- Make facile connection across length scales
- Model sputter growth of "real" multiple layer materials
- Simultaneous experiment/theory feedback
- New materials by non-equilibrium processes.

B
- Thermoelectrics, battery electrode materials, magnets, superconductors, topological insulators ....
- Process control
- Rapidly accelerate development of new thin films for a variety of technologies
Science push: Product development

If we could do ______A_____, materials product engineers would be able to ______B____.

- Validated, open source codes with workflow control
- Find a cubic superconductor with $T_c > 100K$, large $J_c$
- Design/control metal insulator transitions with external control
- Design surface binding of small molecules
- Multi-variate optimisation of materials systems parameters
- Design/predict/fabricate higher soft Bs magnets
- Higher Bs hard magnets
- Modeling finite temperature properties of real materials.
- Annealing behavior of materials

- Accelerated in house design. Will generate jobs.
- 77K magnets and lightweight motors, and magnet cables, low cost.
- New sensor, logic and memory devices; better cathodes.
- Catalysts, biofuels, metal-air batteries, methane conversion
- Simplify materials choices, would reduce time and cost to product production.
- increase HDD density 10x with current head technology
- rare-earth magnet replacement
Delivery mechanism (how do we do it?)

- First do no harm/moderation in all things
- Mini hubs (how to organized? Project focused or platform focused? Materials focused? Not instrument focused? Vertically integrated?)
  - Materials design centers
  - Network of science focused (NSF?)/materials focused(BES?)/technology focused (NIST) and vertically integrated(EERE/DOD)
  - Need more funding for fundamental materials exploration and discovery
  - Software/method development centers – integrate BES/ASCR user facilities?
- Mechanism for open source software development/support
- Real-time theory/simulations at user facilities
- Meta data/ data capture from user facilities
- Mechanism for data capture from existing and published work
- “Google materials” free-access “social media” for materials scientists