Breakout Report on Correlated Materials

Identification of Grand Challenges

Breakout - correlated materials

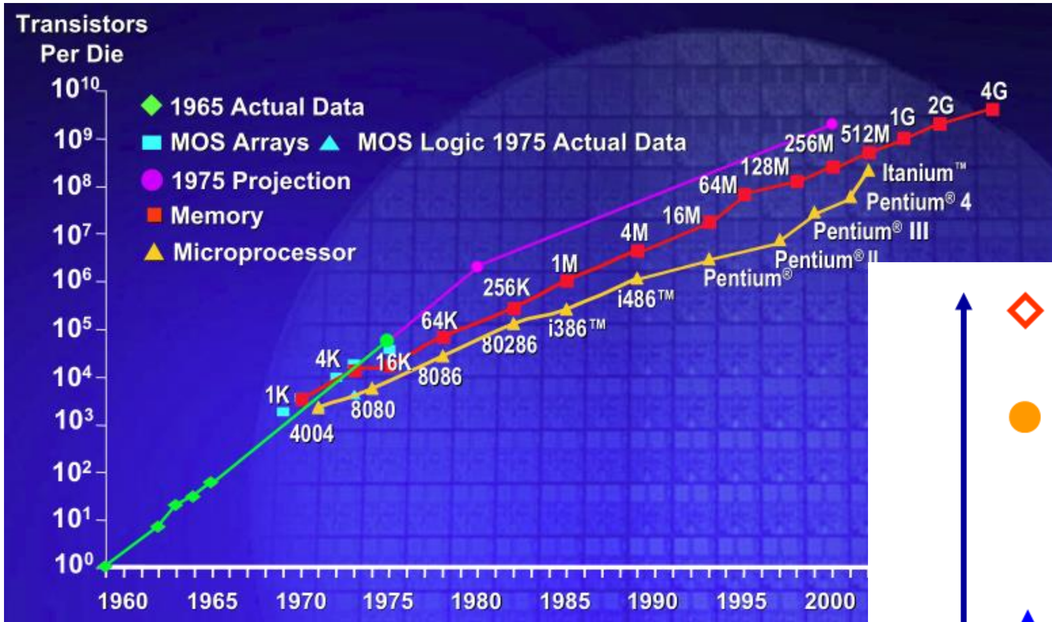
- Chairs: Littlewood (Argonne), Parkin (IBM)
- Speakers: Terris (HGST), Kotliar(Rutgers)

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

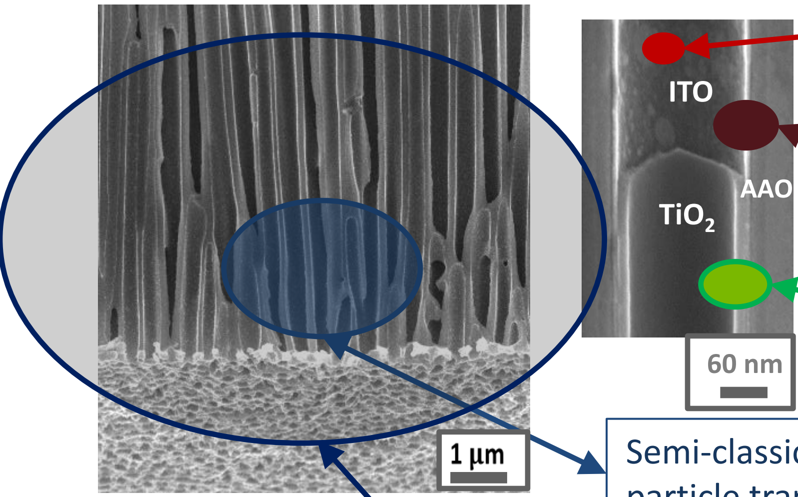
△ Li_2MXO_4 / Gr-Si
Discovery of path to reversible multi-electron cathode material with 4V cell voltage
Market entry > 2017

■ 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

Excited state calculations for electron transfer and photon-mediated transitions

Accurate intermolecular potentials to model structure and dynamics on nanoscale

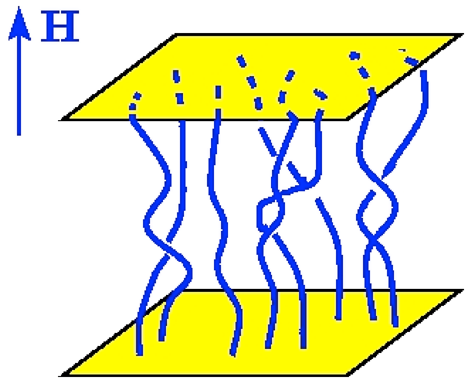
Semi-classical models of electrical and particle transport on mesoscale

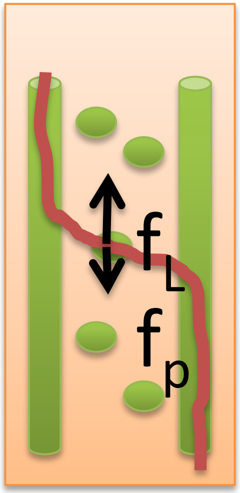
Effective theories of inhomogeneous media: elastic, fluid and electrical transport

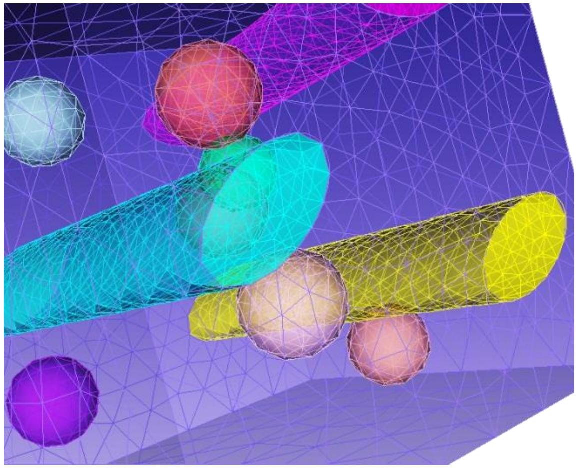
- Each box requires new investment in methods, theory and computation
- Joining up the boxes is as important as the investment in any single piece
- We must curate both data and software
- Design choices driven by application target

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







$$\mathcal{F}_{\mathrm{GL}} = \frac{1}{2}\int d^d x \left\{ \beta\left(\frac{\alpha}{\beta} + |\psi|^2\right)^2 + \frac{\hbar^2}{m}\left|\left(i\nabla - \frac{2\pi}{\phi_0}\mathbf{A}\right)\psi\right|^2 + \frac{1}{4\pi}(\nabla\times\mathbf{A} - \mathbf{H})^2 \right\}$$

Time-dependent Ginzburg -Landau eqn.

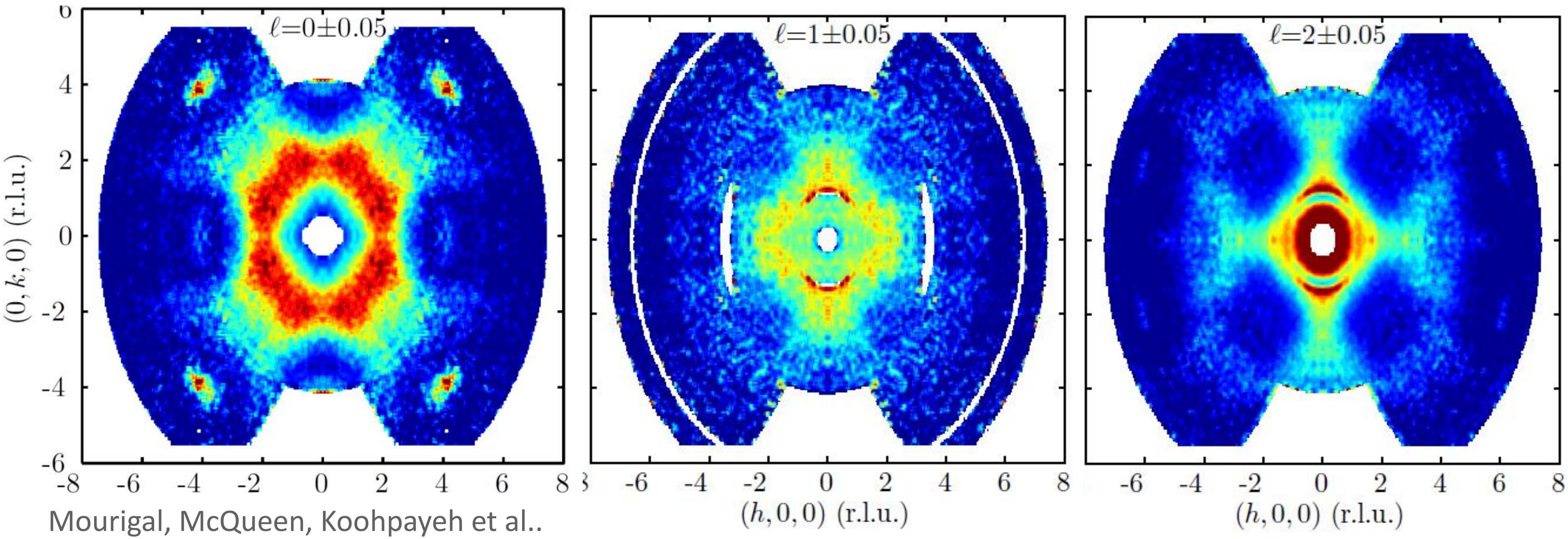
$$\frac{\partial\Psi}{\partial t} = -\frac{\delta\mathcal{F}_{\mathrm{GL}}}{\delta\Psi^*}, \quad \frac{\delta\mathcal{F}_{\mathrm{GL}}}{\delta\mathbf{A}} = 0$$

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”

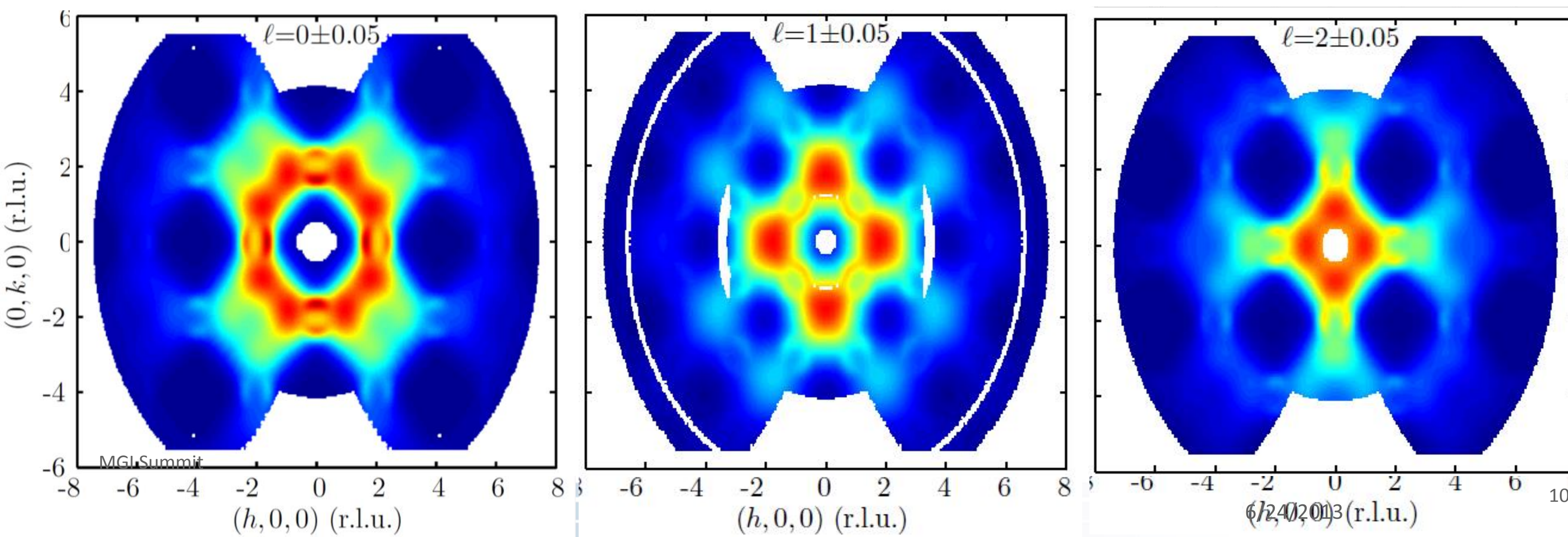
Spin fluctuations in a quantum paramagnet (Collin Broholm)



Mourigal, McQueen, Koohpayeh et al..

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 J_1 (Chalker and Conlon)

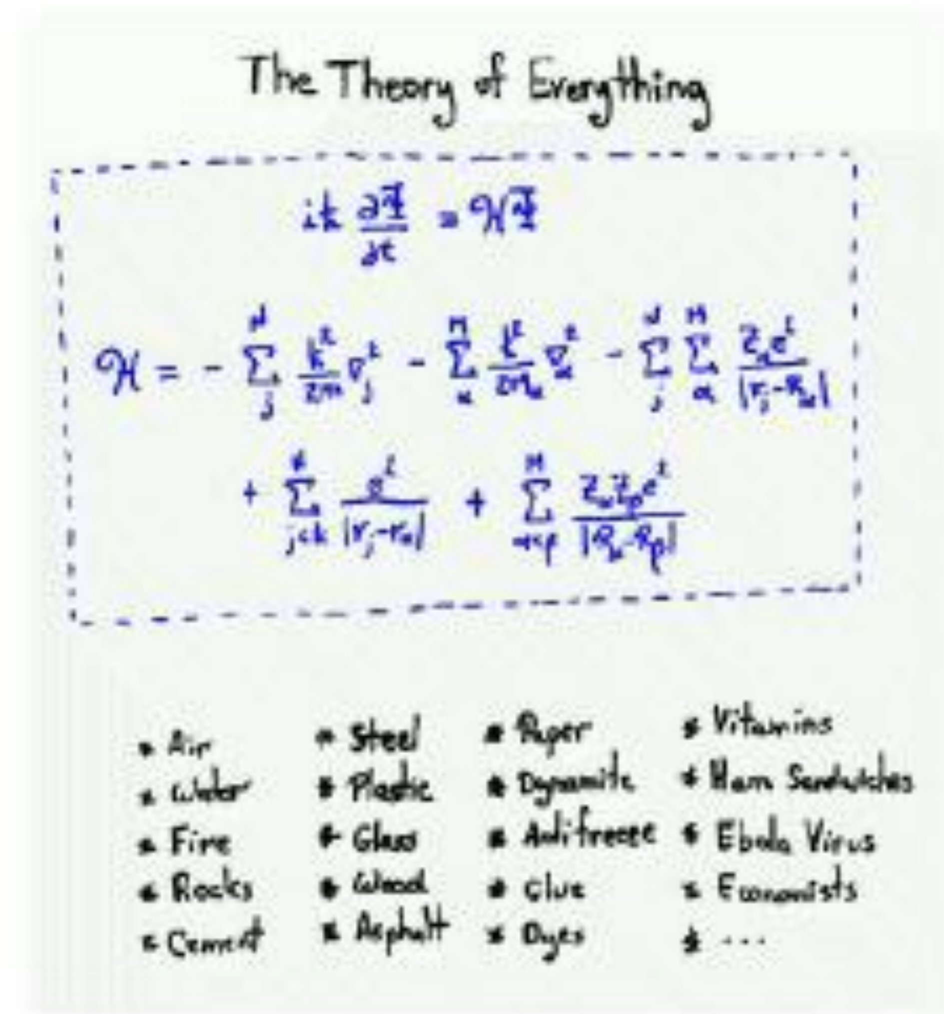


Building multiscale models via “genomics”

Materials by design: genomics?

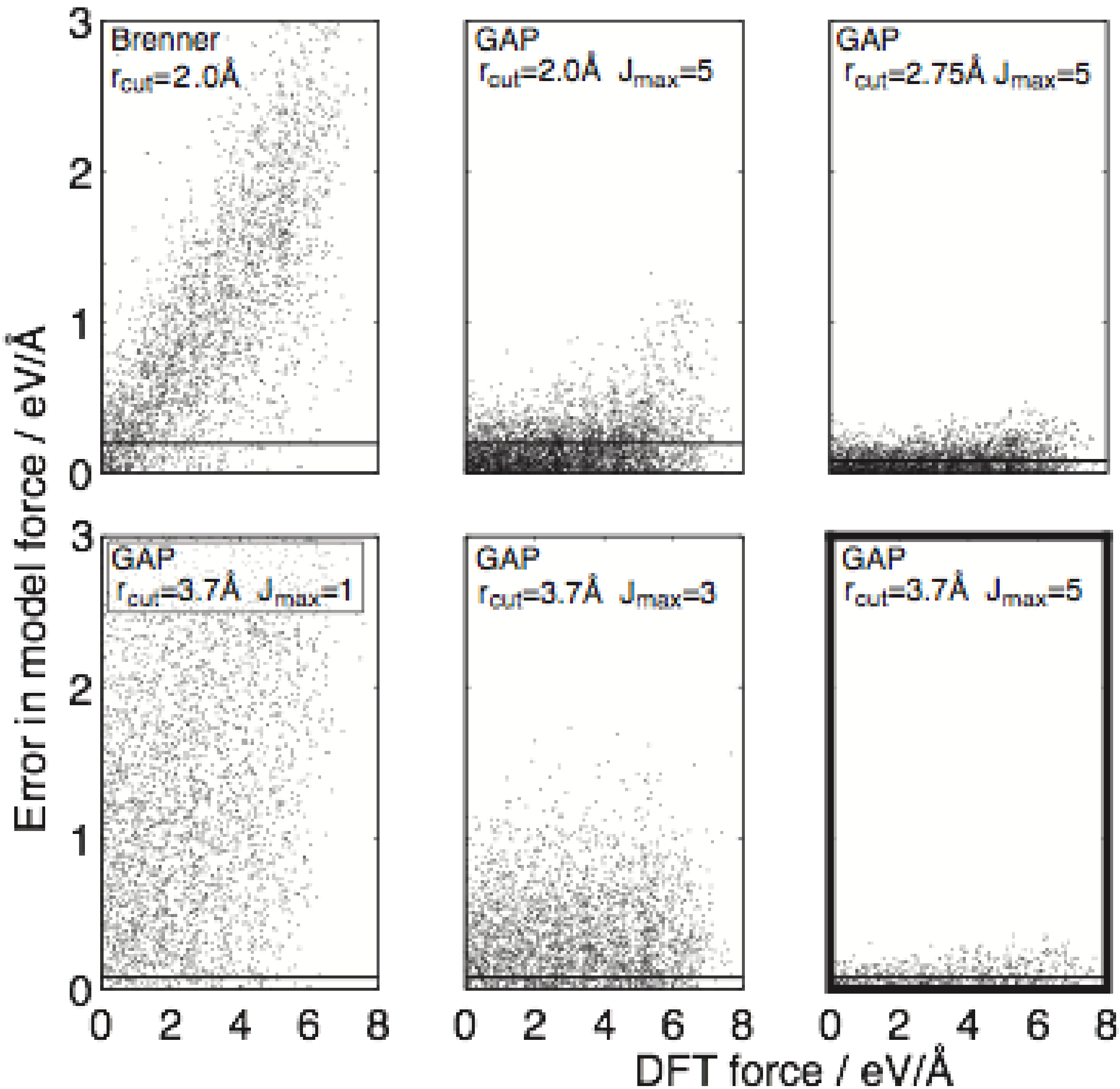
Genomics must be grounded in theory: the human genome initiative depends fundamentally on the “central dogma” of DNA coding. This is both the fundamental **theory** of biology and an **algorithm**

Materials genomics derives its validity from the Schrodinger equation – but this is not (yet) an instruction set



Robert Laughlin (Nobel lecture)

Supervised learning: Gaussian Approximation Potentials trained on DFT (Gabor Csanyi)



Diamond (1000 K)

Theoretical limit for given cutoff: RMS of long range forces

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
- Materials-specific informed scale-bridging.
- 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