Cornell University

"I would found an institution where any person can find instruction in any study."
− Ezra Cornell, 1868

Advanced Materials

Perspective from the frontiers of complex oxide materials by design

Craig J. Fennie
School of Applied and Engineering Physics
fennie@cornell.edu

Engineering College Council Meeting, October 30, 2015

Advanced Materials Approach: Take home message

Obama and Feynman

Only through Ezra's vision can we realize ...

Advanced Materials

Perspective from the frontiers of complex oxide materials by design

1. The Need – "Materials-by-Design"
2. Our Vision – closing the loop between theory & experiment, science & engineering
3. How it is working at Cornell! – Advance Materials example, complex oxides
4. Centers we brought in to help support our vision
5. Potential next steps

Advanced Materials

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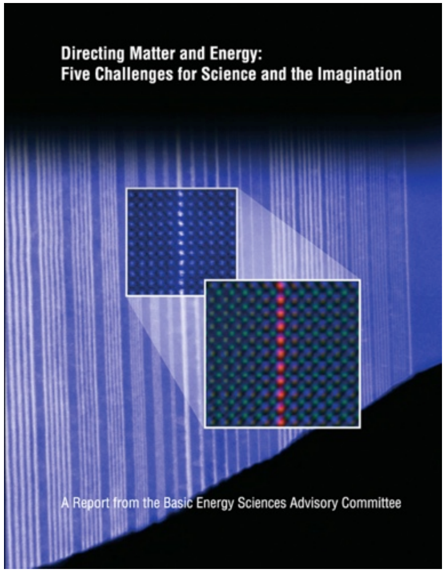
The DOE: Atomic-scale Materials by Design, a national grand Challenge

In this new era of science, design, discover, and synthesize new materials and molecular assemblies at the levels of electrons and atoms

The collective efforts of condensed matter and materials physicists, chemists, biologists, molecular engineers, and those skilled in applied mathematics and computer science.

Directing Matter and Energy: Five Challenges for Science and the Imagination (DOE BESAC 2007)



A. Ohtomo, D.A. Muller, J.L. Grazul, and H.Y. Hwang *Nature* **419** (2002) 378-380.

The National Research Council: Single Crystal Bulk Materials Discovery is a national need

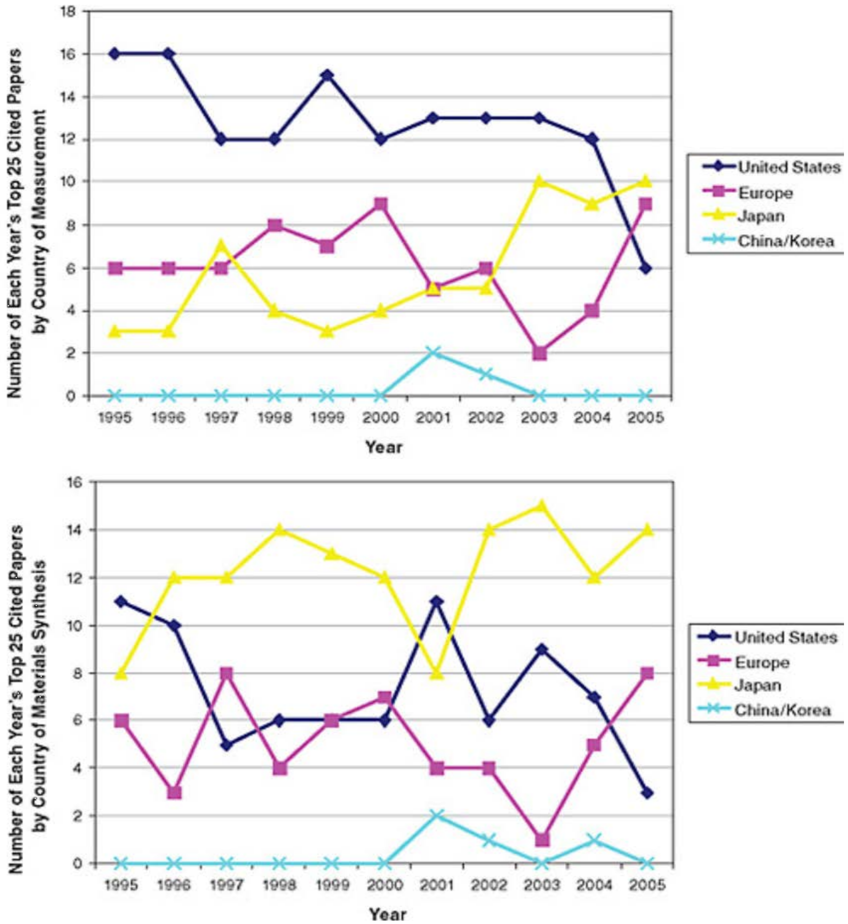
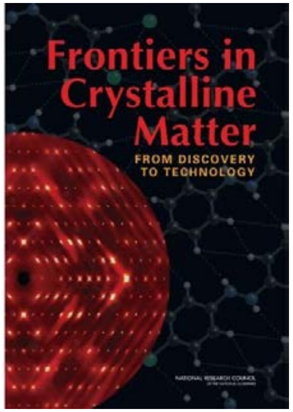


FIGURE 3.6 Country of origin of the 25 most highly cited papers in superconductivity by year, 1995 through 2005, distinguished by country of measurement (top) and country of materials synthesis (bottom).

Characterization of Superconductors (Top-Cited Papers)

Synthesis of Superconductors (Top-Cited Papers)

Frontiers in Crystalline Matter: From Discovery to Technology (National Research Council, 2009) p. 107.



Materials Genome Initiative

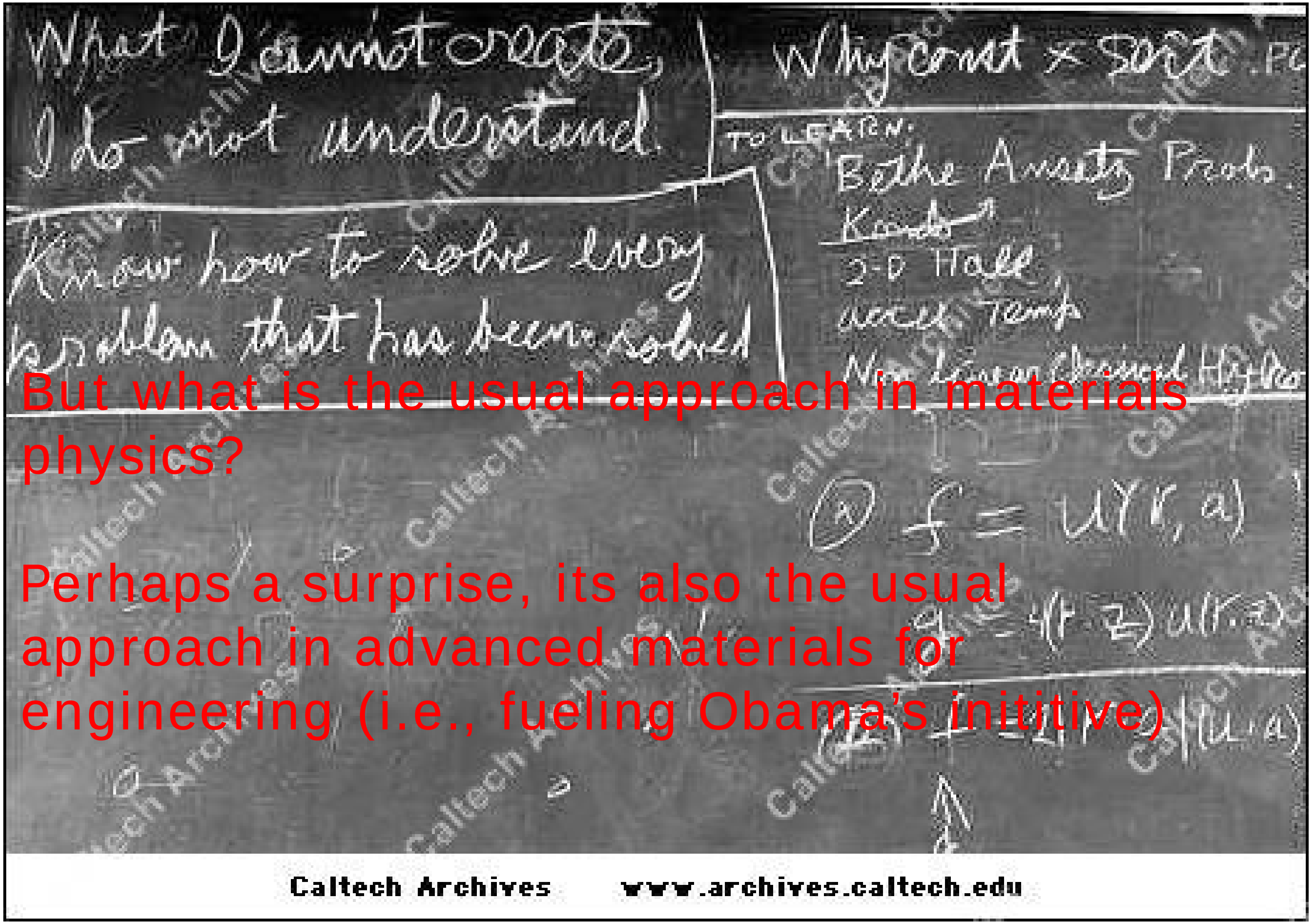
Discover, develop, manufacture, and deploy advanced materials at least twice as fast as possible today, at a fraction of the cost

June 30, 2011 at Carnegie-Mellon Univ.

*"The only solution is **materials and chemistry by design**, using new synthesis and characterization tools, theory, and simulation and modeling to understand complex materials and chemical systems and predict the most promising research directions."*

Computational Materials Science and Chemistry for Innovation, DOE (2010)

Feynman's last blackboard



But what is the usual approach in materials physics?

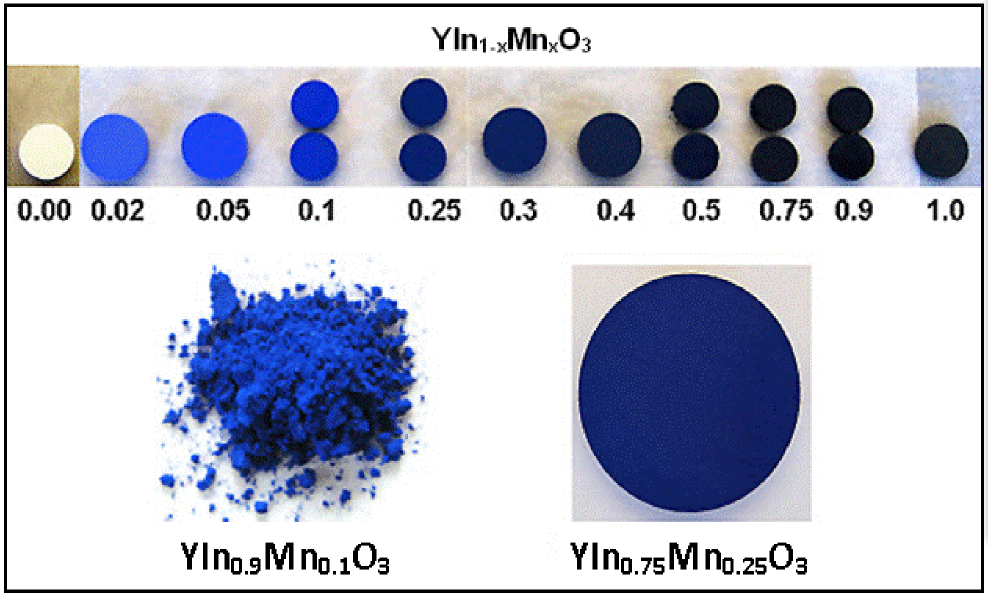
Perhaps a surprise, its also the usual approach in advanced materials for engineering (i.e., fueling Obama's inititive)

The challenge of materials design / discovery

The New York Times

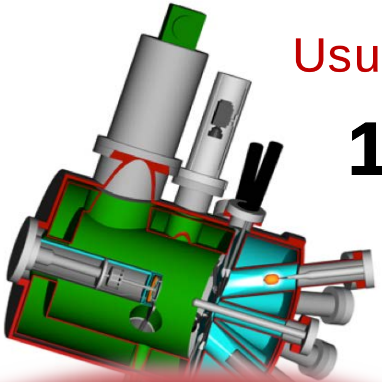
By Happy Accident, Chemists Produce a New Blue

By KENNETH CHANG
Published: November 23, 2009



Mas Subramanian, Oregon State
Going after an enhanced multiferroics

Advanced Materials: Usual Approach



Usually guided by intuition alone

1. Synthesize

Create Useful Materials
(Engineering side)

Study Fundamental Interactions
(Science side)

2. Characterize

3. Compare with targeted metric
(and occasionally with theory)

3. Describe microscopically
(i.e., Theory)

Advanced Materials

Perspective from the frontiers of complex oxide materials by design

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2. Our Vision – closing the loop between theory & experiment, science & engineering

3. How it is working at Cornell! – Advance Materials example, complex oxides

4. Centers we brought in to help support our vision

5. Potential next steps

Advanced Materials: We break the rules

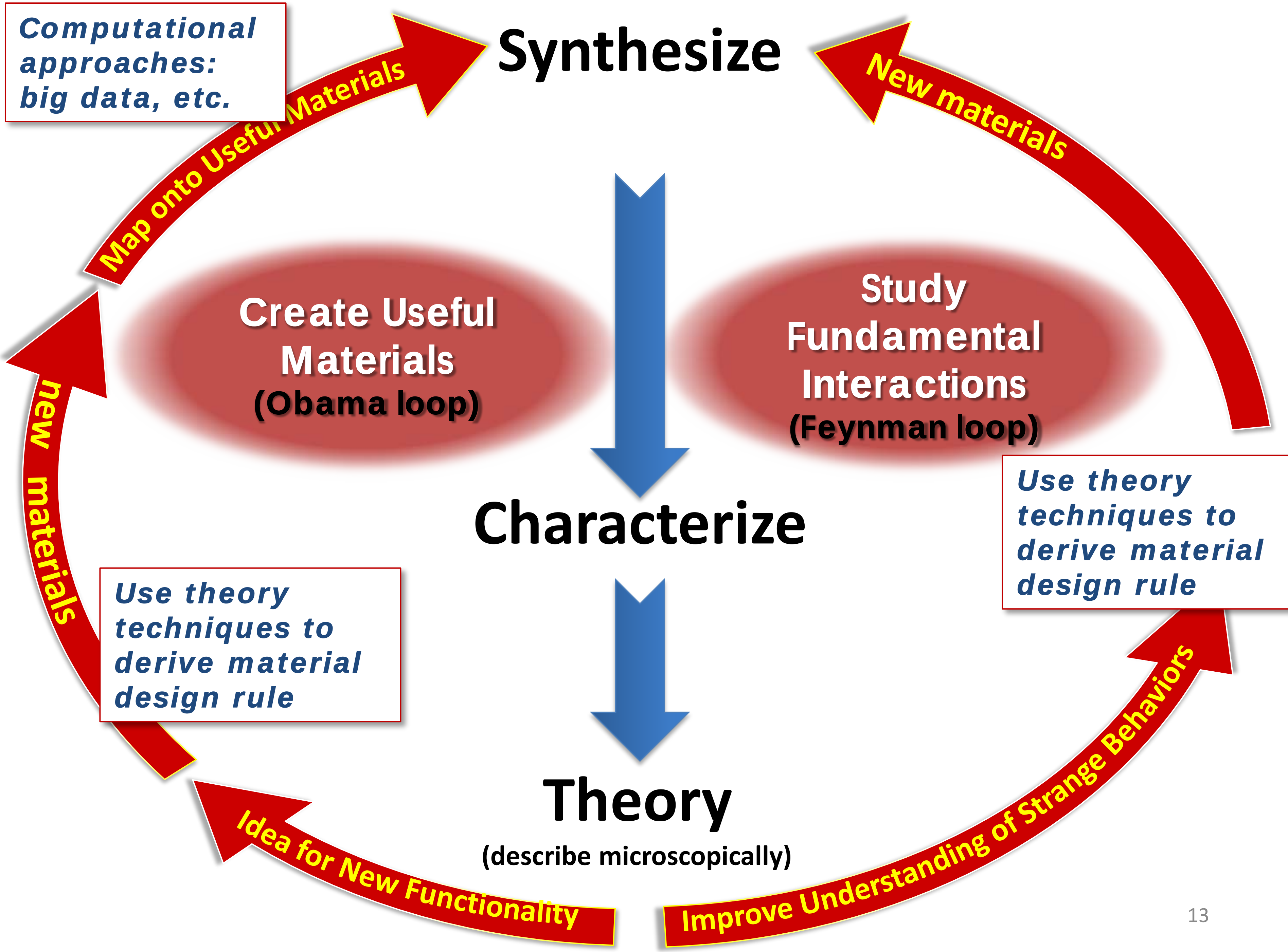
Perspective from the frontiers of complex oxide materials by design

We just don't break one rule, we break all the rules

Rule 1: Fundamental science and applied science (engineering) do not "speak" to each other

Rule 2: Theory "supports" experiment

Rule 3: Theoretical physicists and chemists don't belong in engineering



Synthesize
Computational approaches: big data, etc.
Map onto Useful Materials
New materials
Create Useful Materials (Obama loop)
Study Fundamental Interactions (Feynman loop)
new materials
Characterize
Use theory techniques to derive material design rule
Use theory techniques to derive material design rule
Theory
(describe microscopically)
Idea for New Functionality
Improve Understanding of Strange Behaviors

Advanced Materials

Perspective from the frontiers of complex oxide materials by design

Advanced Materials encompasses many types of materials for many different applications.

- I'm now going to focus on Complex oxides
- And focus only on *new materials* for electronic and magnetic devices

Advanced Materials

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4. e

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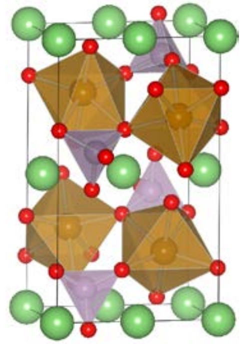
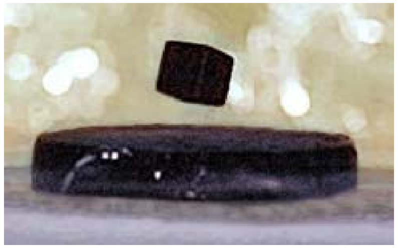
6. Potential next steps

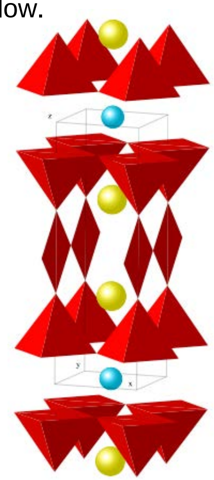
A High Resolution Transmission Electron Microscopy image of a $BaTiO_3/SrTiO_3$ superlattice grown by Molecular Beam Epitaxy [Schlom, et al. J. Am. Cer. Soc. **91** 2429 (2008)].
J. Heber, Nature **459** 28 (2009)



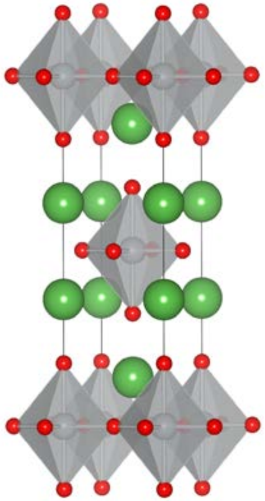
Electric vehicles like the Nissan Leaf are powered by Li-ion batteries. $LiFePO_4$ (right) is being actively researched as a next-generation cathode material for Li-ion batteries.



High-temperature superconductivity was first discovered in a layered oxide material. The structure of the superconductor $YBa_2Cu_3O_{7-\delta}$ is shown below.

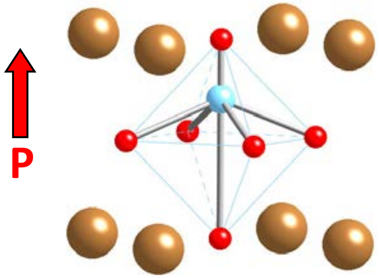


An Energy Server (manufactured by Bloom Energy), a power generator that uses Solid Oxide Fuel Cells.



Right: The structure of La_2NiO_4, a mixed ionic-electronic conductor being studied for potential application as a cathode in intermediate temperature Solid Oxide Fuel Cells.

A ferroelectric random access memory chip from Ramtron (and Texas Instruments, below)



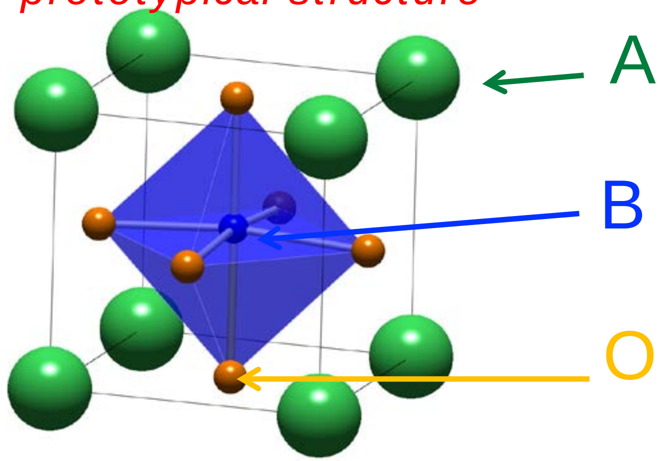
A ferroelectric distortion in the perovskite oxide $PbTiO_3$, one of the materials used in FeRAM devices. The arrow shows the direction of the electrical polarization.

Oxides and oxide-like materials are important to many different areas of science and society, from fundamental science to electronic devices and clean energy technologies

“More is Different,” Phil Anderson, Science 1972

Complex oxides: ABO_3 Perovskites

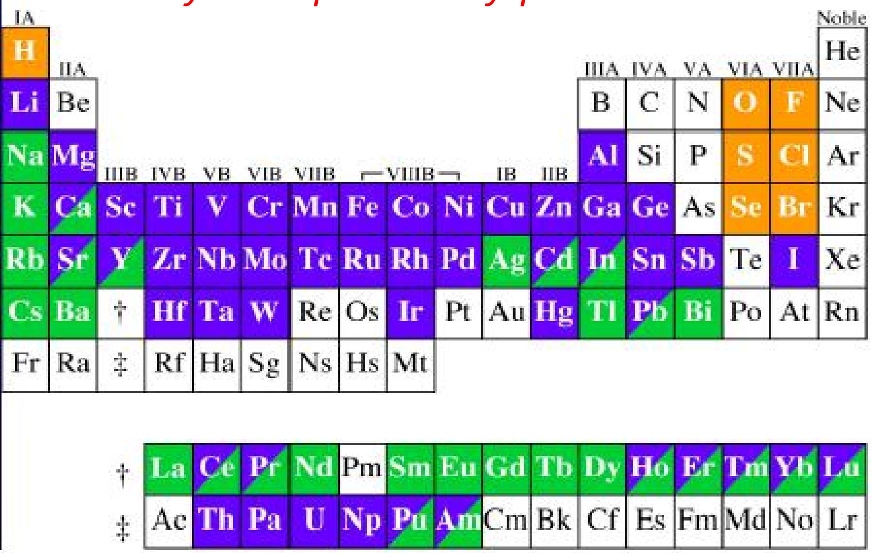
Same prototypical structure



Nearly any physical property

- Dielectric $CaTiO_3$, $SrTiO_3$, $(CaCu_3)(Ti_4)(O_4)_3$
- Ferroelectric $BaTiO_3$, $LiNbO_3$, $PbTiO_3$
- Magnetoelectric $TbMnO_3$, $BiFeO_3$
- Antiferroelectric $PbZrO_3$
- Piezoelectric $PbZr_xTi_{1-x}O_3$
- Antiferromagnetic $LaMnO_3$
- Ferromagnetic $SrRuO_3$
- Superconducting doped-$SrTiO_3$
- Colossal Magneto-resistance $(La,Ca)MnO_3$

Challenge and opportunity: Enormous number of tertiary and quaternary perovskites



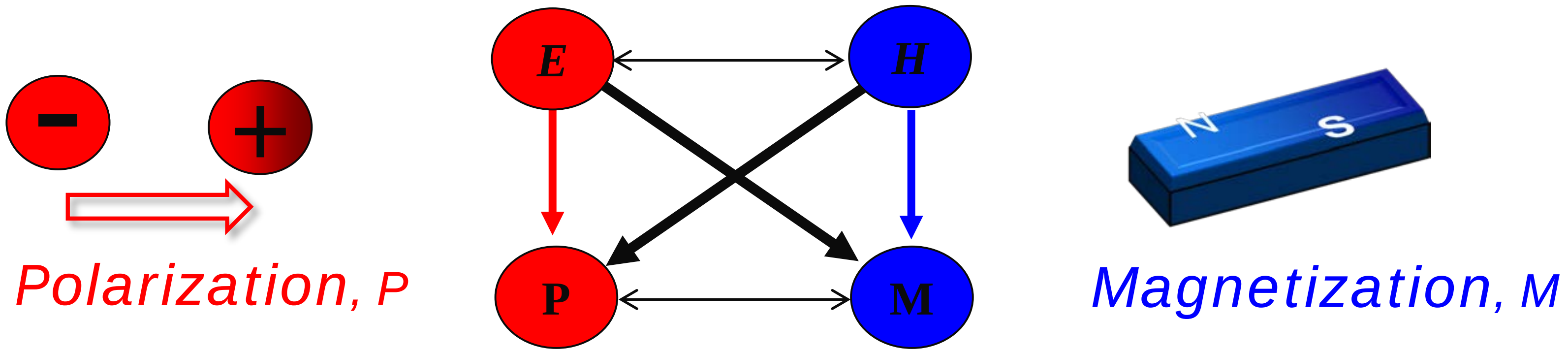
Advances in synthesis and characterization - tailoring properties at the atomic-scale

$(LaMnO_3)_{2n}(SrMnO_3)_n$

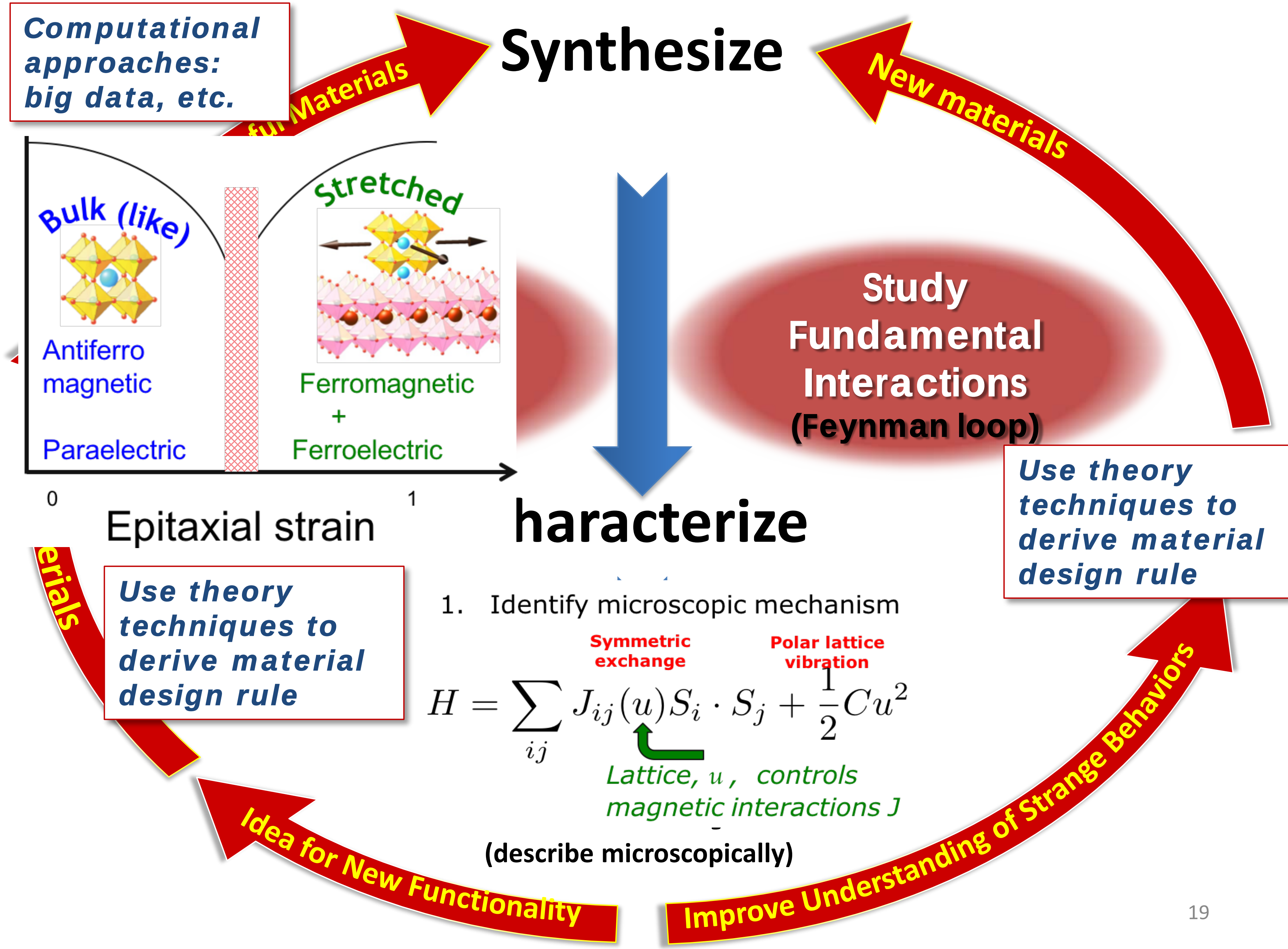
Monkman, …Schlom, Muller, & Kyle Shen (Nature Materials 2012)

An example: Multiferroics

(Generalized) **Magnetoelectric**: cross coupled response to electric and magnetic fields

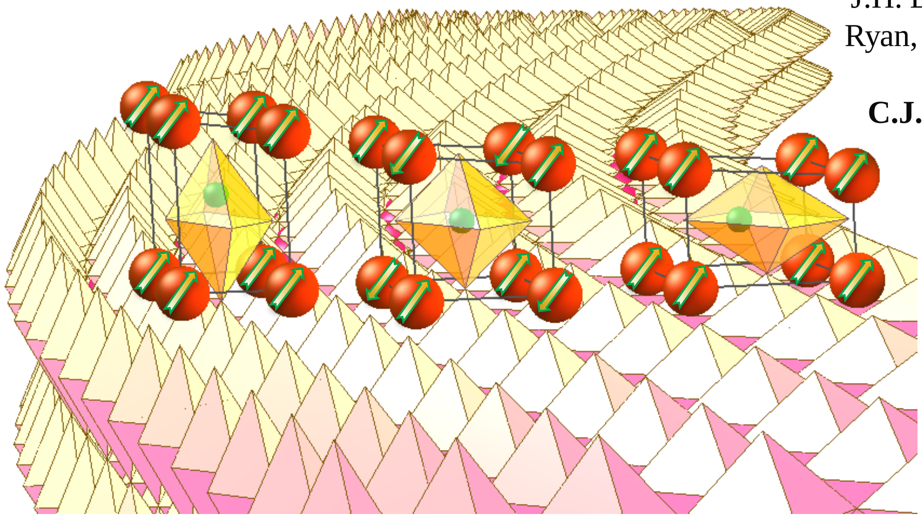


i.e. control of the magnetic **M** *(electric* **P***) phase with an applied electric* ***E*** *(magnetic* ***H****) field*

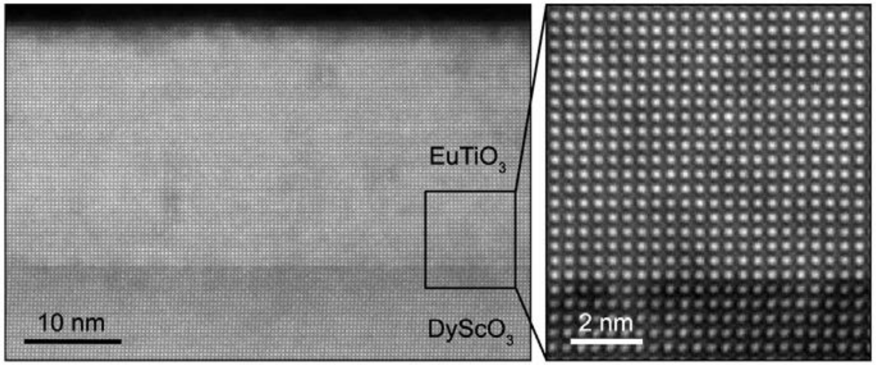


Computational approaches: big data, etc.
Synthesize
ful Materials
New materials
Bulk (like)
Stretched
Antiferro magnetic
Paraelectric
Ferromagnetic + Ferroelectric
0
1
Epitaxial strain
Study Fundamental Interactions (Feynman loop)
haracterize
Use theory techniques to derive material design rule
erials
Use theory techniques to derive material design rule
1. Identify microscopic mechanism
Symmetric exchange
Polar lattice vibration
$H = \sum_{ij} J_{ij}(u) S_i \cdot S_j + \frac{1}{2} C u^2$
Lattice, u, controls magnetic interactions J
(describe microscopically)
Idea for New Functionality
Improve Understanding of Strange Behaviors

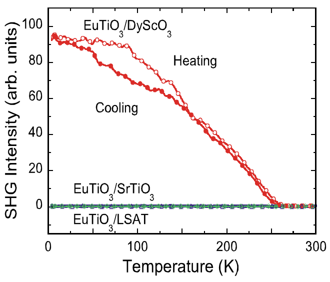
Strongest Ferromagnetic Ferroelectric



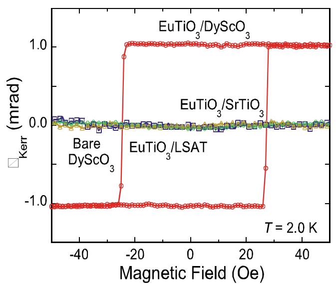
J.H. Lee, L. Fang, E. Vlahos, X. Ke, Y.W. Jung, **L.F. Kourkoutis**, J-W. Kim, P.J. Ryan, T. Heeg, M. Roeckerath,V. Goian, M. Bernhagen, R. Uecker, P.C. Hammel, K.M. Rabe, S. Kamba, J. Schubert, J.W. Freeland, **D.A. Muller**, **C.J. Fennie**, P. Schiffer, V. Gopalan, E. Johnston-Halperin, and **D.G. Schlom**,
Nature **466** (2010) 954-958.

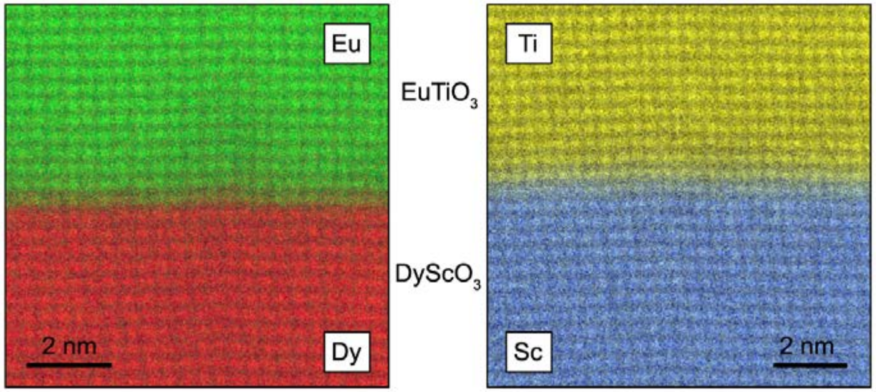


Ferroelectric
P ~ 20 μC/cm2



Ferromagnetic
~ 5 μ_B/Eu





22 nm thick $EuTiO_3$ (a boring dielectric) + 1.1% Strain (by growing it commensurately) = Multiferroic (1000× stronger than prior ferromagnetic ferroelectrics)

Why Cornell !

In the words of Hans Bethe, we have an unfair advantage

Leverages Cornell's Facilities

- CCMR
- CHESS
- STEM Facility
- Cryo-STEM
  (NSF-MRI Award $2.7 M) <= Lena Kourkoutis, AEP
- MBE + ARPES <= Kyle Shen, Physics

Why Cornell !: Our approach to materials discovery requires …

In the words of Hans Bethe, we have an unfair advantage, no boundaries …

Students trained to be experts in physics, chemistry, or materials science (etc) …

- *yet are trained to work with and understand the the issues of one or more of the other fields*

e.g., I need physics theory students (from the physics dept), but I train them in material chemistry and materials science and how and how to work closely with experimentalists and engineers.

"I would found an institution where any person can find instruction in any study." − Ezra Cornell,

Advanced Materials takes a village (and patience)

In the words of Hans Bethe, we have an unfair advantage

1.

Theory discovery* (2006)

Craig J. Fennie & Karin M. Rabe
Physical Review Letters

Experiment confirmation (2010)

J.H. Lee, L. Fang, E. Vlahos, X. Ke, Y.W. Jung, **L.F. Kourkoutis**, J-W. Kim, P.J. Ryan, T. Heeg, M. Roeckerath,V. Goian, M. Bernhagen, R. Uecker, P.C. Hammel, K.M. Rabe, S. Kamba, J. Schubert, J.W. Freeland, **D.A. Muller**,**C.J. Fennie**, P. Schiffer, V. Gopalan, E. Johnston-Halperin, and **D.G. Schlom**, *Nature* **466** (2010) 954-958.

2.

Theory discovery* (2011)

Turan Birol & **Craig J. Fennie**
Physical Review Letters

Experimental confirmation and more (2013)

C.H. Lee, N.D. Orloff, T. Birol, Y. Zhu, V. Goian, E. Rocas, R. Haislmaier E. Vlahos, J.A. Mundy, **L.F. Kourkoutis**, Y. Nie, M.D. Biegalski, J. Zhang M. Bernhagen, N.A. Benedek, Y. Kim, J.D. Brock, R. Uecker, X.X. Xi, V. Gopalan, D. Nuzhnyy, S. Kamba**, D.A. Muller**, I. Takeuchi, J.C. Booth, **C.J. Fennie, and D.G. Schlom**, *Nature* **502** (2013) 532-536.

3.

Theory discovery* (2011)

Nicole A. Benedek & C.J. Fennie
Physical Review Letters

Experiment (2015)

not at cornell, need bulk synthesis

1. Experimental confirmation and more (**bulk single crystals**)
   S-W Cheong, Rutgers; *Nature Materials, 2015*
2. Experimental confirmation (**bulk**)
   Matt Rosensky, Liverpool; *Science, 2015*

** New physics, new functionality, and the material realization*

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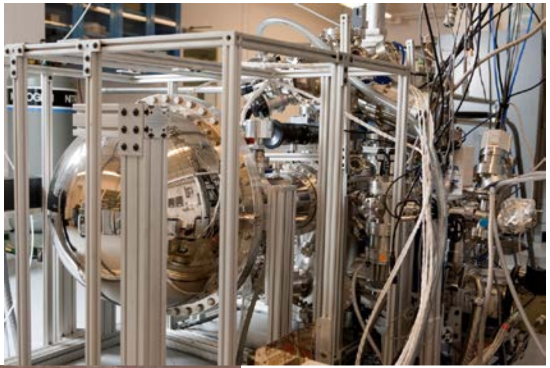
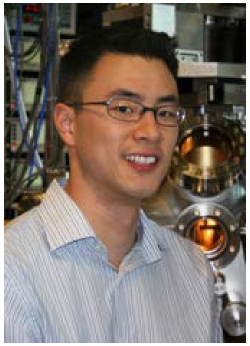
Why Cornell !: The Team (characterization)

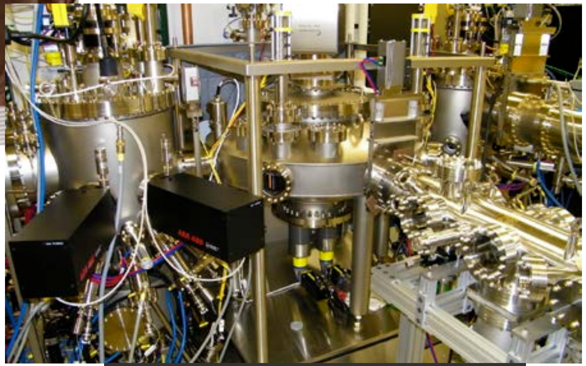
- Electron Microscopy
  - David Muller (AEP)
  - Lena Kourkoutis (AEP)
- Synchrotron Diffraction
  - Joel Brock (AEP)
- Angle-Resolved Photoemission
  - Kyle Shen (Physics)
- Spectroscopic-Imaging STM
  - Séamus Davis (Physics)



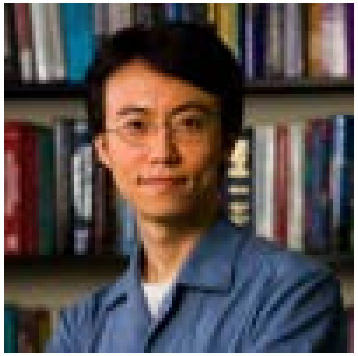




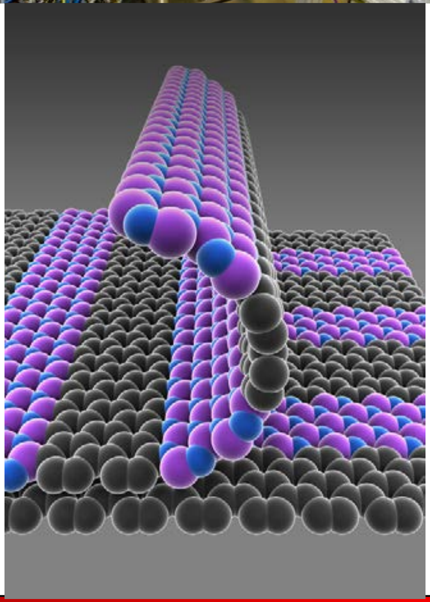
Why Cornell !: The Team (synthesis)

- Molecular-Beam Epitaxy
  Darrell Schlom (MSE)



- Synthesis of 2d materials
  Jiwoong Park (Chemistry)





Why Cornell !: The Team (theory; inorganic correlated phenomena)

- **Craig Fennie (AEP)**
  Materials Design inorganic materials, Physics of insulators

Associate Professor

- **Eun-Ah Kim (Physics)**
  models relevant to materials in which electron correlations are key

Associate Professor

Phase I—Moore Foundation

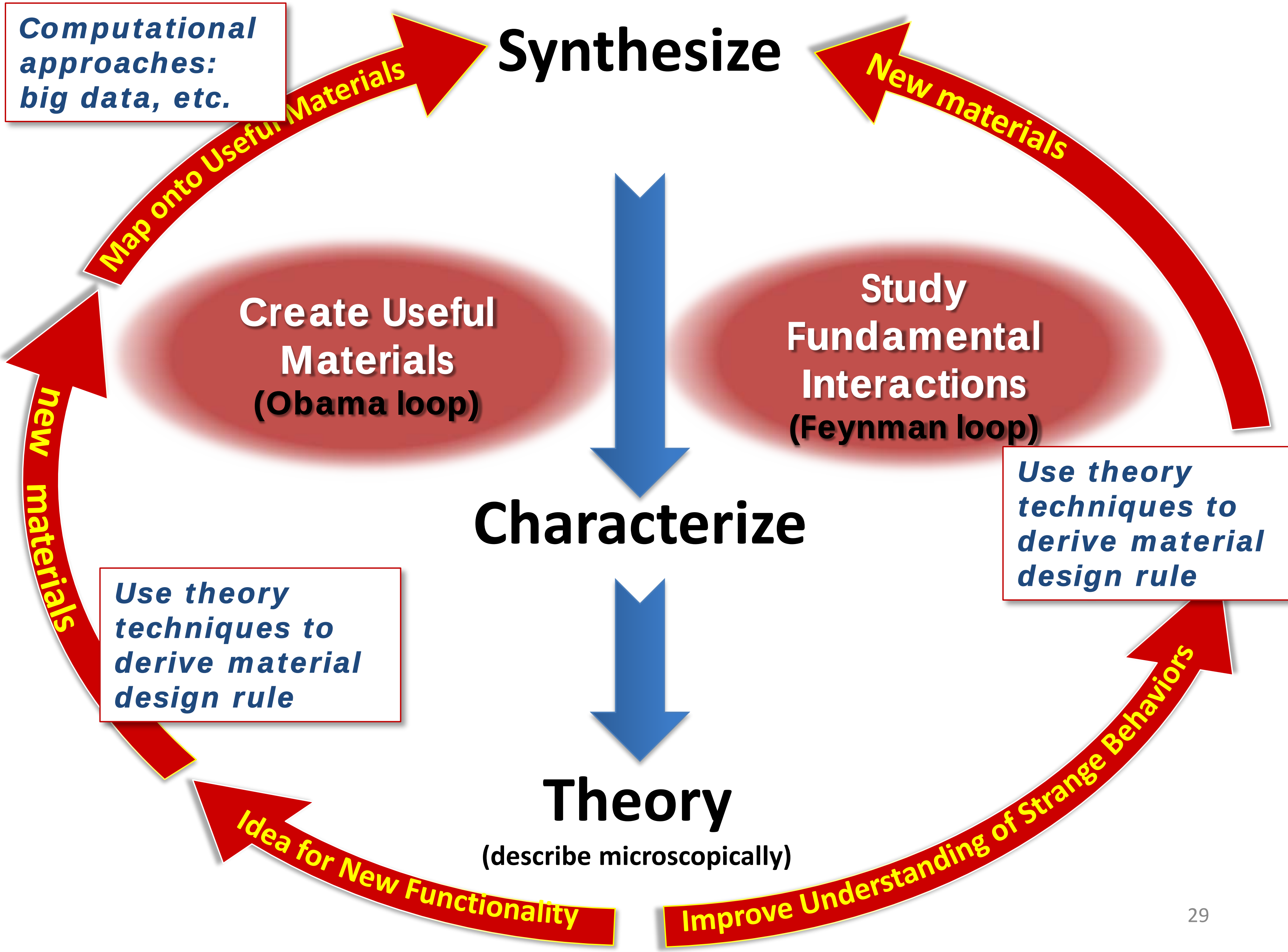
Emergent Phenomena in Quantum Systems (EPiQS)

GORDON AND BETTY MOORE FOUNDATION

Search

To fuel discovery and conceptual breakthroughs, the EPiQS initiative will support:

- Top experimentalists and centers for theory to enable current and emerging leaders in experiment and theory to maximize their creativity
- Materials synthesis to bolster the artistry of creating new/better quantum materials while improving career paths for scientists
- Instrumentation acquisition and development to advance lab capabilities at leading institutions
- High-risk projects to enable timely responses to new discoveries and development of new concepts
- Community building activities that create and sustain a vibrant research network to promote the exchange of ideas and materials


Computational approaches: big data, etc.
Map onto Useful Materials
Synthesize
New materials
Create Useful Materials
(Obama loop)
Study Fundamental Interactions
(Feynman loop)
Characterize
Use theory techniques to derive material design rule
new materials
Use theory techniques to derive material design rule
Theory
(describe microscopically)
Idea for New Functionality
Improve Understanding of Strange Behaviors

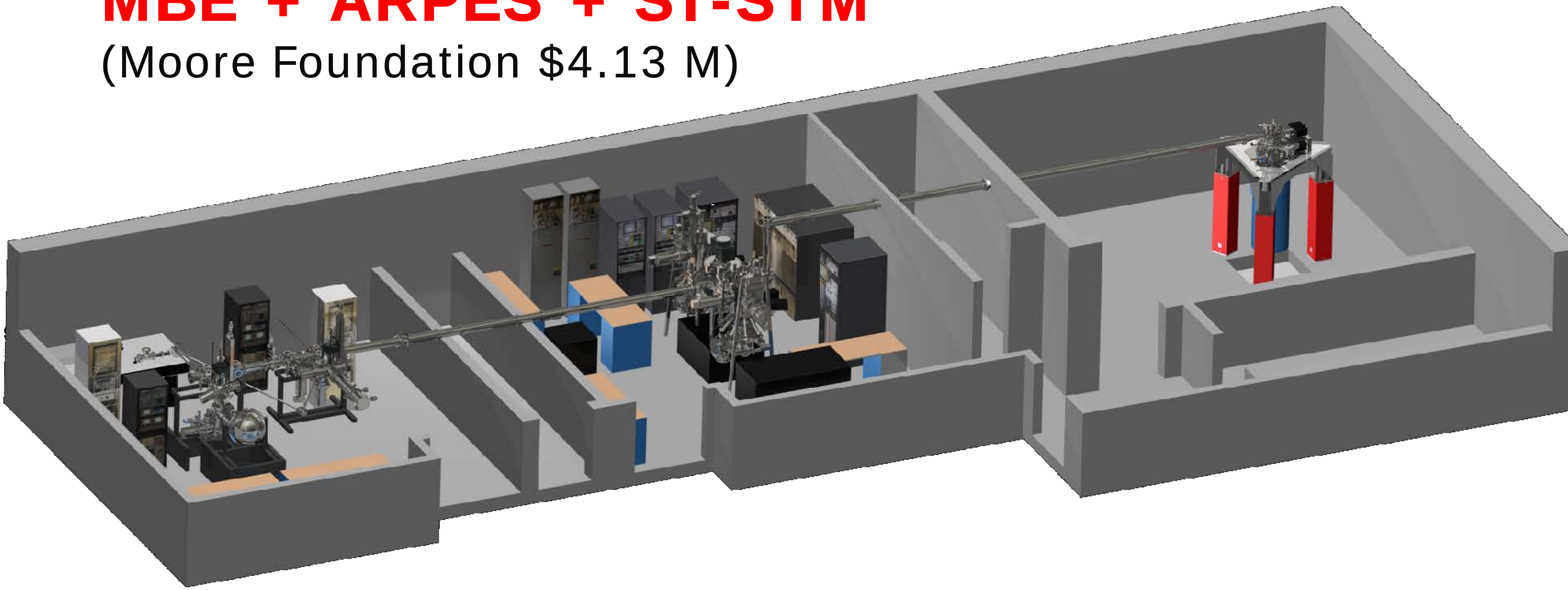
Moore money: Instrumentation development

Emergent Phenomena in Quantum Systems (EPiQS)

The first (and only)

MBE + ARPES + SI-STM

(Moore Foundation $4.13 M)



Moore money: Experimental single investigators

Emergent Phenomena in Quantum Systems (EPiQS)

The selected *Experimental Investigators in Quantum Materials* are:

- Peter Abbamonte, University of Illinois at Urbana-Champaign
- Dimitri Basov, University of California at San Diego
- Collin Broholm, Johns Hopkins University
- Jak Chakhalian, University of Arkansas
- J. C. Séamus Davis, Cornell University
- Nuh Gedik, Massachusetts Institute of Technology
- M. Zahid Hasan, Princeton University
- Tony Heinz, Stanford University
- Jennifer Hoffman, Harvard University
- Pablo Jarillo-Herrero, Massachusetts Institute of Technology
- Aharon Kapitulnik, Stanford University
- Philip Kim, Harvard University
- Margaret Murnane, University of Colorado
- Nai Phuan Ong, Princeton University
- Joseph Orenstein, University of California at Berkeley
- Jason Petta, Princeton University
- Zhi-Xun Shen, Stanford University
- Amir Yacoby, Harvard University
- Ali Yazdani, Princeton University

Moore money: Postdoctoral Theory Scholar Centers

Emergent Phenomena in Quantum Systems (EPiQS)

EPiQS Funding to Boost Quantum Materials Theory Research at Six Universities

- Harvard University
- Massachusetts Institute of Technology
- Stanford University
- University of California at Berkeley
- University of California at Santa Barbara
- University of Illinois at Urbana-Champaign

We will provide about $8 million over five years through these six awards. The grants will support Moore Postdoctoral Theory Scholars for appointments of up to three years and Moore Visiting Scholars for appointments ranging from a few months to one year. We anticipate that about 25 postdoctoral scholars will be trained and about a dozen visiting scholars will be hosted within this grant portfolio.

Profs Eun-ah Kim (physics) and Craig Fennie (AEP) were invited to submit a proposal during this round

(two years ago, both kim and Fennie were Assistant professors)

- the feedback we received as to why we did not win, we don't have the track record of producing faculty
- since then ...

Phase II—NSF

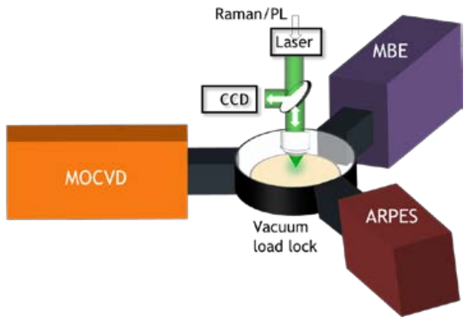
Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM)

- $25M / 5 years
- Flagship—Cornell leads first "platform" in this new NSF program
- User Facilities
  - Theory (Clark Atlanta University + Cornell)
  - Bulk Crystal Growth (Johns Hopkins)
  - Characterization (Cornell)
  - Thin Film Growth (Cornell)

Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM)

In-House Research Program

Creating Interface Materials with Designed Properties



ACTIVE SUBSTRATE + THIN FILM

New Chemistry
New Physics
New Materials Science

User Facility

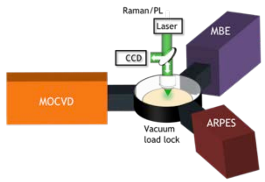
Accelerating the pace at which new bulk and thin film crystalline materials are designed, realized experimentally, and measured

CASCADE

Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM)

Creating Interface Materials with Designed Properties

+



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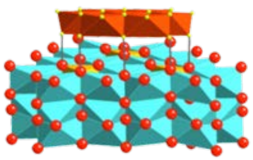
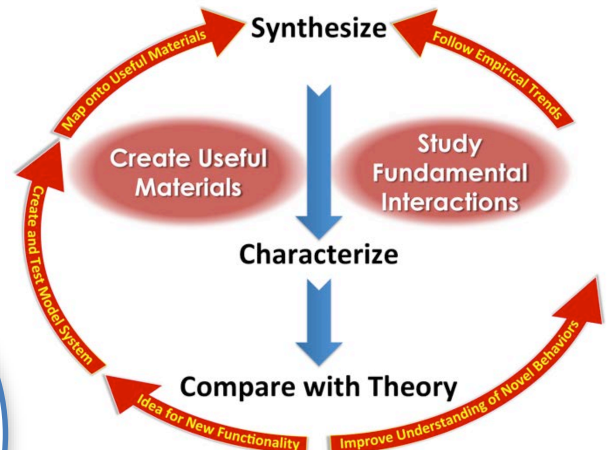
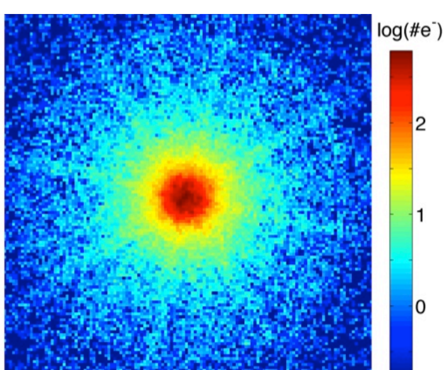


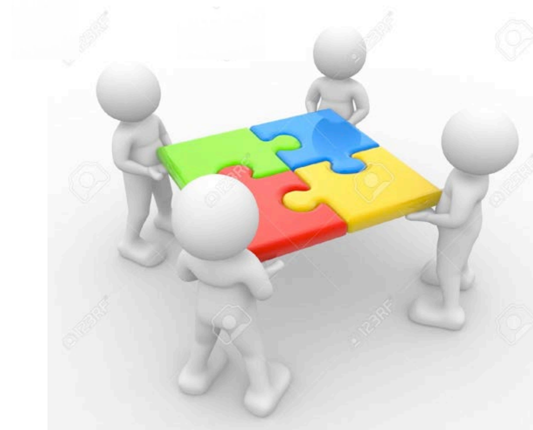
Empowering Users



Developing Novel Instrumentation and Techniques



Training Tomorrow's Technologists



Phase III—ramping this up

- DOE-EFRC (2016?)

- Moore Foundation
  (EPiQS round #2, program monitor says planning to kick-off $100 million program in 2018)

Additional Benefits

- Spin-Off Effects (Cornell will have the jewels first)
  - Novel Properties will Feed Device efforts in THz, Non-Linear Optics, Spintronics, Sensors, MEMS, new types of Transistors, ... (ECE, AEP, MAE)
  - Interactions with Cornell NYTech, Corning, Start-ups ...
- Intellectual Property for Cornell
- Fits Advanced Materials Strategic Objective of COE
- Fundamental—excellent fit with Cornell
- Makes Cornell Mecca for New Materials
- Fuels “Break the Rules” Innovations at Cornell
- Scalable as Initiative (and Cornell leadership) takes off

Advanced Materials

Perspective from the frontiers of complex oxide materials by design

1. The Need – "Materials-by-Design"
2. Our Vision – closing the loop between theory & experiment, science & engineering
3. How it is working at Cornell! – Advance Materials example, complex oxides
4. Centers we brought in to help support our vision
5. Potential next steps

Next Steps: Theory Postdoctoral center

Moore and the NSF made a gigantic investment in capital equipment, but not a similar investment in theory capitol, i.e., people.

- We need bright young theory pd's to take advantage of these investments.
- Cornell could seed a Theory Postdoctoral center related to these centers (administered by the Cornell Kavli Center: Kavli will match the contribution)
  - To accelerate our track record of producing new faculty – Fennie has so far placed 1 student and 2 pd's in tenure track faculty positions at peer institutions (U Minn, UT-Austin, and Seoul National) and one DOE National Lab (Ames)
  - Create a pool of candidates for theory positions in Engineering at Cornell
  - *Note: this is NOT a money grab for my group, it would be run by Kavli, decisions made by a panel of experts (theorists, and more importantly, experimentalists!!)*
- Eventually expand to include the entire college, every material class

e.g., Princeton realized about 10 years ago, that they have more theoretical physicists in engineering than in Physics, they created a prestigious Engineering Theory Postdoctoral Fellowship program.

There is a critical need to expand theory faculty in engineering at Cornell

Theory faculty vs total faculty at the top 10 MSE programs

US News & World report ranking	Theorists	Total Faculty
1. MIT	7	40
2. UCSB	4	28
3. Northwestern	7	44
4. Stanford	1	18
4. UIUC	4	24
6. Georgia Tech	3	37
6. Berkeley	4	17
8. Cornell	1	17
8. CalTech (MSE/Applied Physics same dept)	4	23
10. Carnegie Mellon	4	26

Data collected by Prof Nicole Benedek, MSE

Next: 5 new theory faculty in engineering in 5 years

In my opinion, the way to think about a faculty hire in theory for advanced materials, this person is an expert in a particular

- *material class (broadly speaking, e.g., complex oxides) and the physics & chemistry & functionality of that class of materials*

Or,

- *device and associated physics (e.g., quantum transport in nanostructures) that could be realized in a variety of material classes*

Don't hire a theorist if they don't know as much about the problem as the leading experimental expert,
i.e., it isnt about the theory/computational tools, its about the science/engineering/ideas

Next: 5 new theory faculty in engineering in 5 years

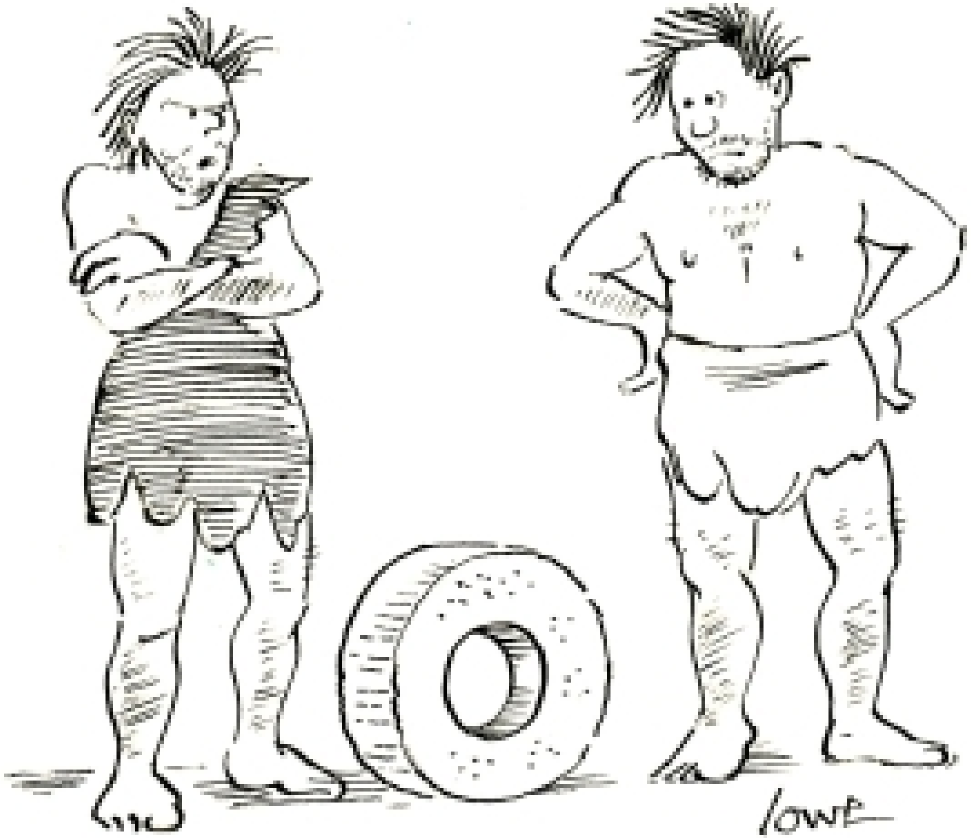
Suggested areas in advanced materials (in order of need)

1. Quantum transport and device physics
2. Polymeric materials (organic, organic/inorganic, etc)
3. Electronic structure of nanostructures
4. Energy applications such as pv, catalysis
5. Biophysics related to the brain (not really advanced materials but it sure is cool)

Don't hire a theorist if they don't know as much about the problem as the leading experimental expert,
i.e., it isnt about the theory/computational tools, its about the science/engineering/ideas

Summary

Typically an engineer's view of science

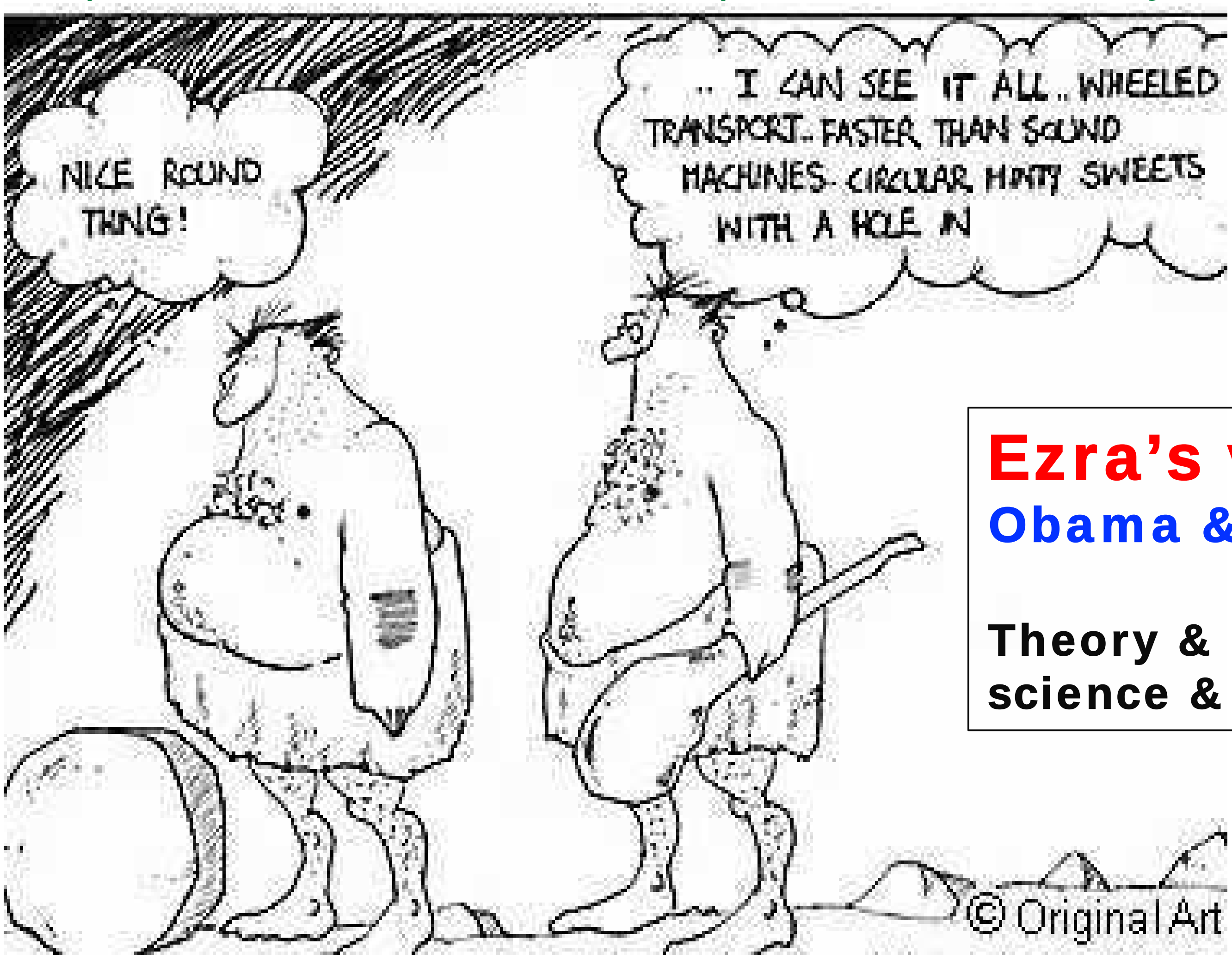


"It doesn't do anything, it's just a very pleasing shape!"

Typically an scientist's view of engineering

Advanced Materials by design: Obama and Feynman

Perspective from the frontiers of complex oxide materials by design



Ezra's vision

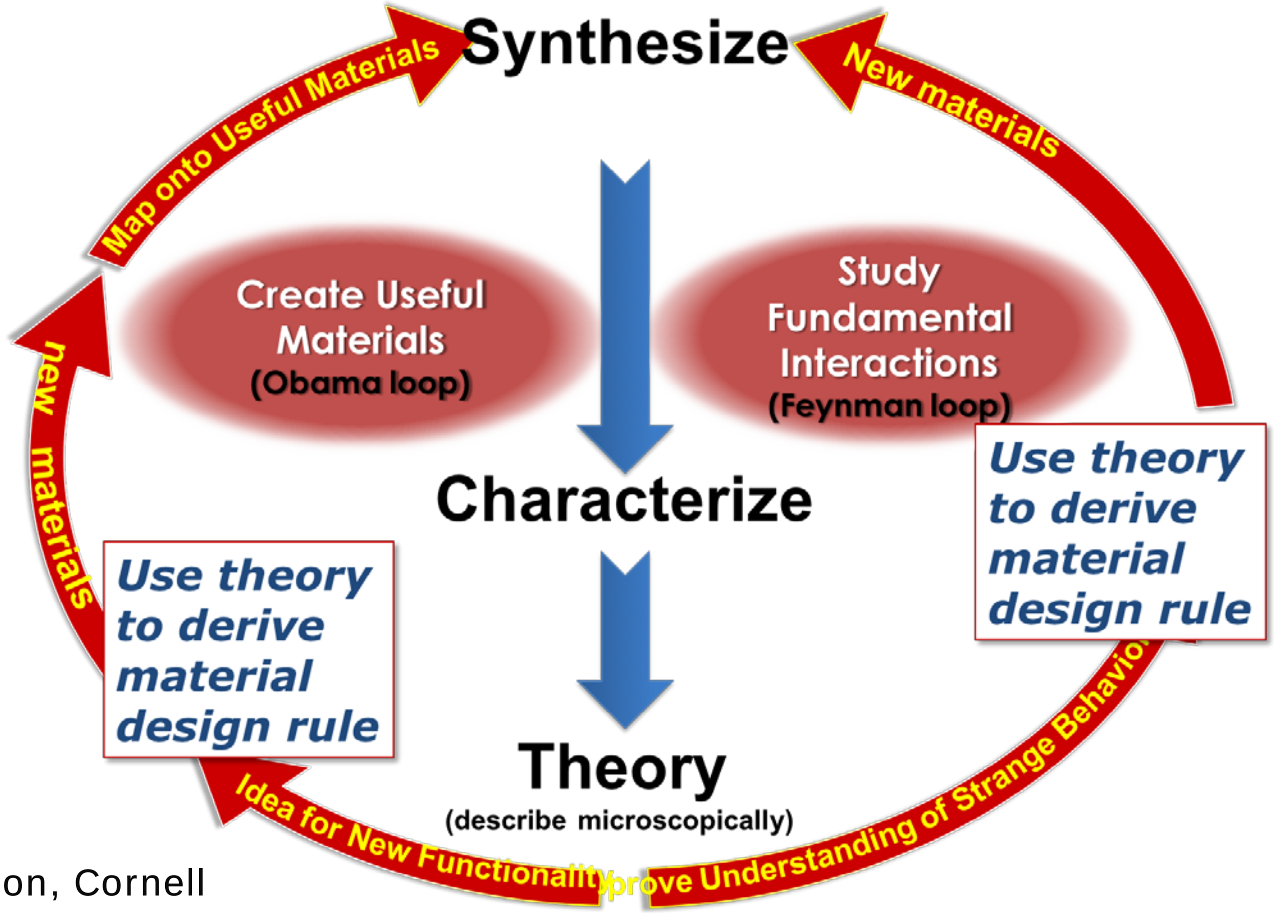
Obama & Feynman

Theory & experiment, science & engineering

Ug was to regret not seeing the potential

The next Obama-Feynman challenge in Complex oxide like materials: new physics for new application directions

For example … photovoltatics



Many needs, but what is clear,

1. *Bulk synthesis expert*
2. *Characterization leader in pv*
3. *Device theorist! (in ECE most likely)*

Regardless of pv is the direction, Cornell engineering needs

1. Device theorist, and an
2. Electronic structure theorist

The next Obama-Feynman challenge: "Organic" materials

For example …
Will Dichtel (Chemistry)
Chris Ober (MSE)
Uli Weisner (MSE)

I'll let the organic experts tell you their needs, but what is clear to me,
Need organic materials theorist!!!