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 20, 2015

Advanced Materials

Perspective from the frontiers of complex oxide materials by design

- The Need – "Materials-by-Design"
- Our Vision – closing the loop between theory & experiment, science & engineering
- Why Cornell! – Advance Materials example, complex oxides
- Centers we brought in to support our vision
- Future possible directions

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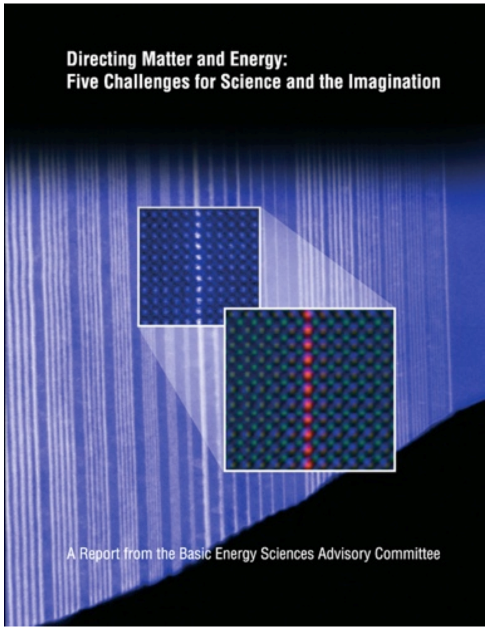
DOE Grand Challenges #1-3

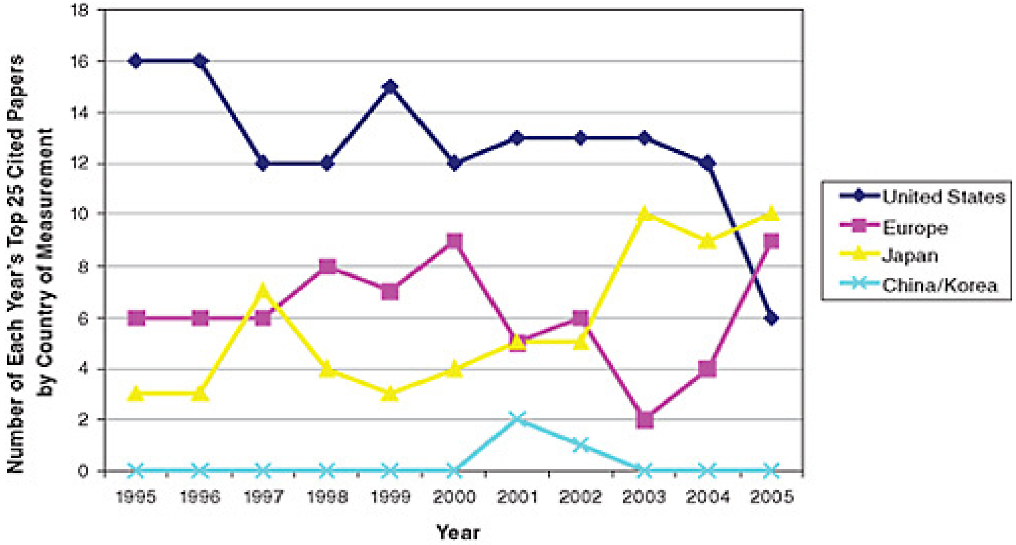
- How do we control material processes at the level of electrons?
- How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties?
- How do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents and how can we control these properties?

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.

Recognized National Need



Characterization of Superconductors (Top-Cited Papers)

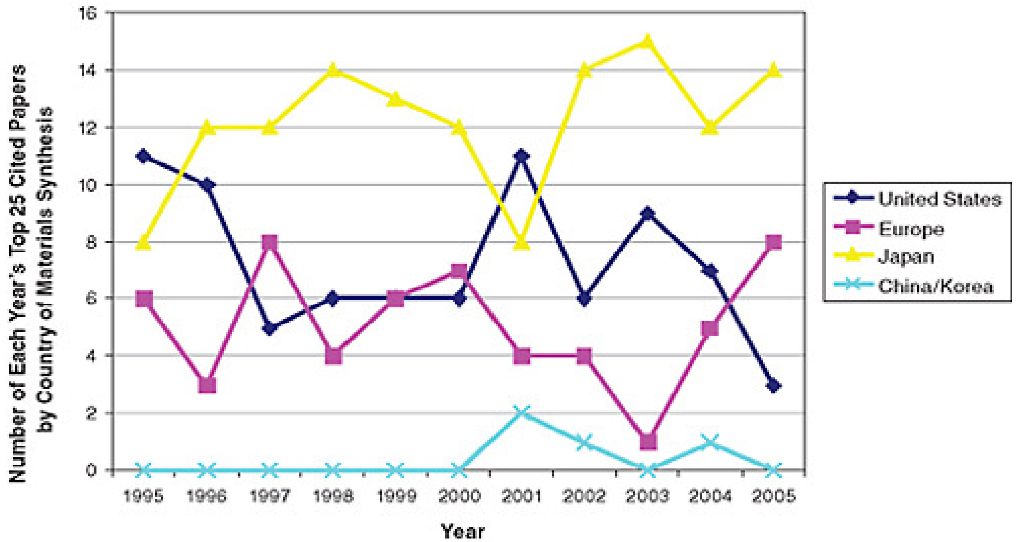
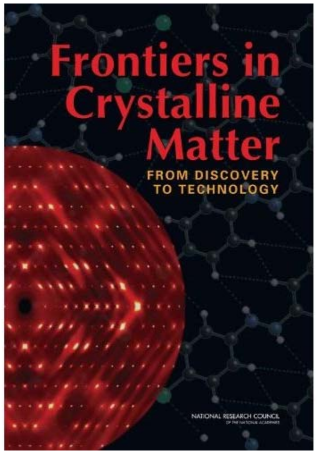


FIGURE 3.6 Country of origin of the 25 most highly cited papers in superconductivity by year, 1995 through 2005, distinguished by country of measurement (top) and country of materials synthesis (bottom).

Synthesis of Superconductors (Top-Cited Papers)

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



Materials Genome Initiative

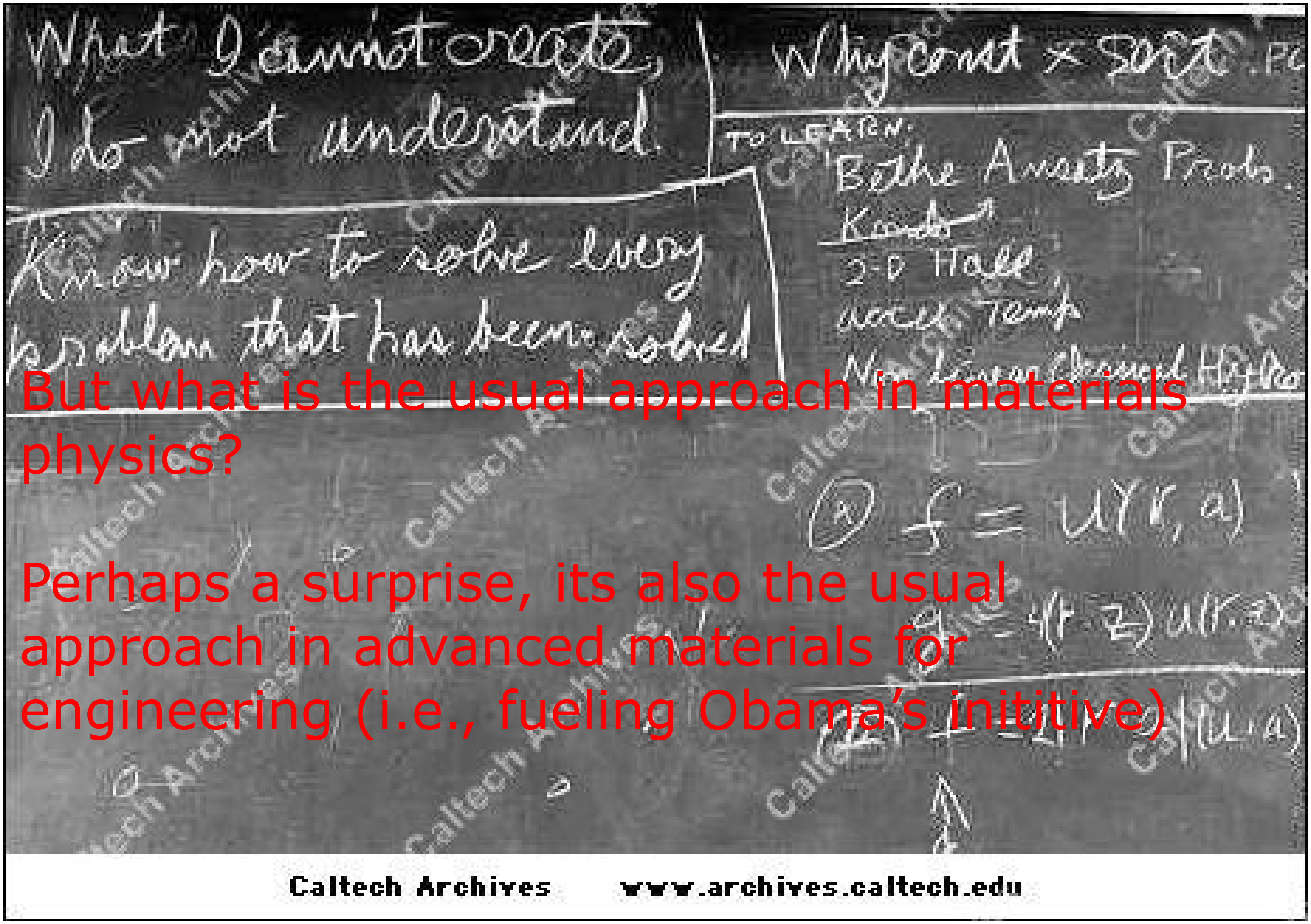
- Discover, develop, manufacture, and deploy advanced materials at least twice as fast as possible today, at a fraction of the cost

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)

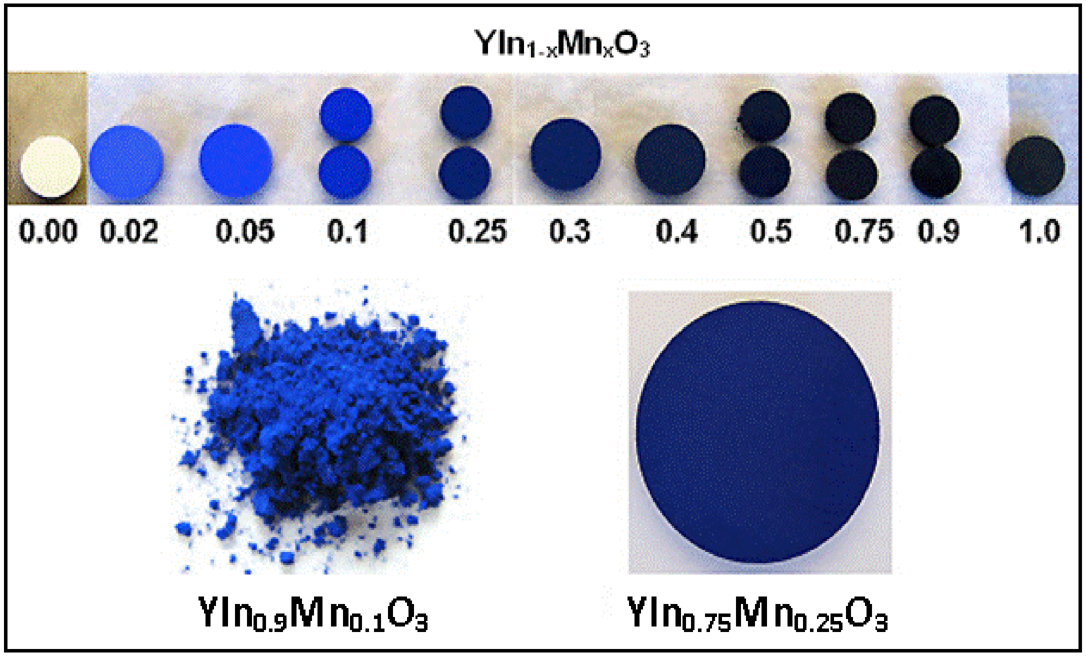
The challenge of materials design / discovery

The New York Times

By Happy Accident, Chemists Produce a New Blue

By KENNETH CHANG

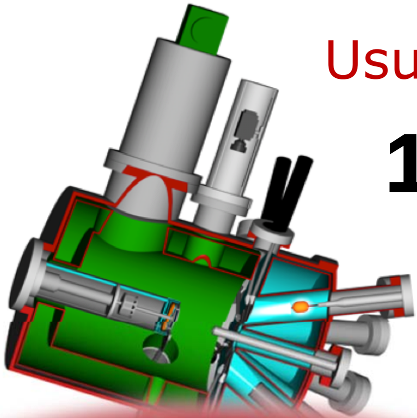
Published: November 23, 2009



Mas Subramanian, Oregon State

Going after an enhanced multiferroics

Advanced Materials: Usual Approach

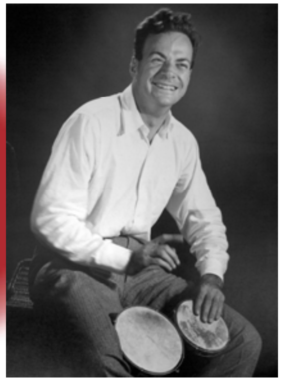


Usually guided by intuition alone

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)

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Advanced Materials: We break the rules

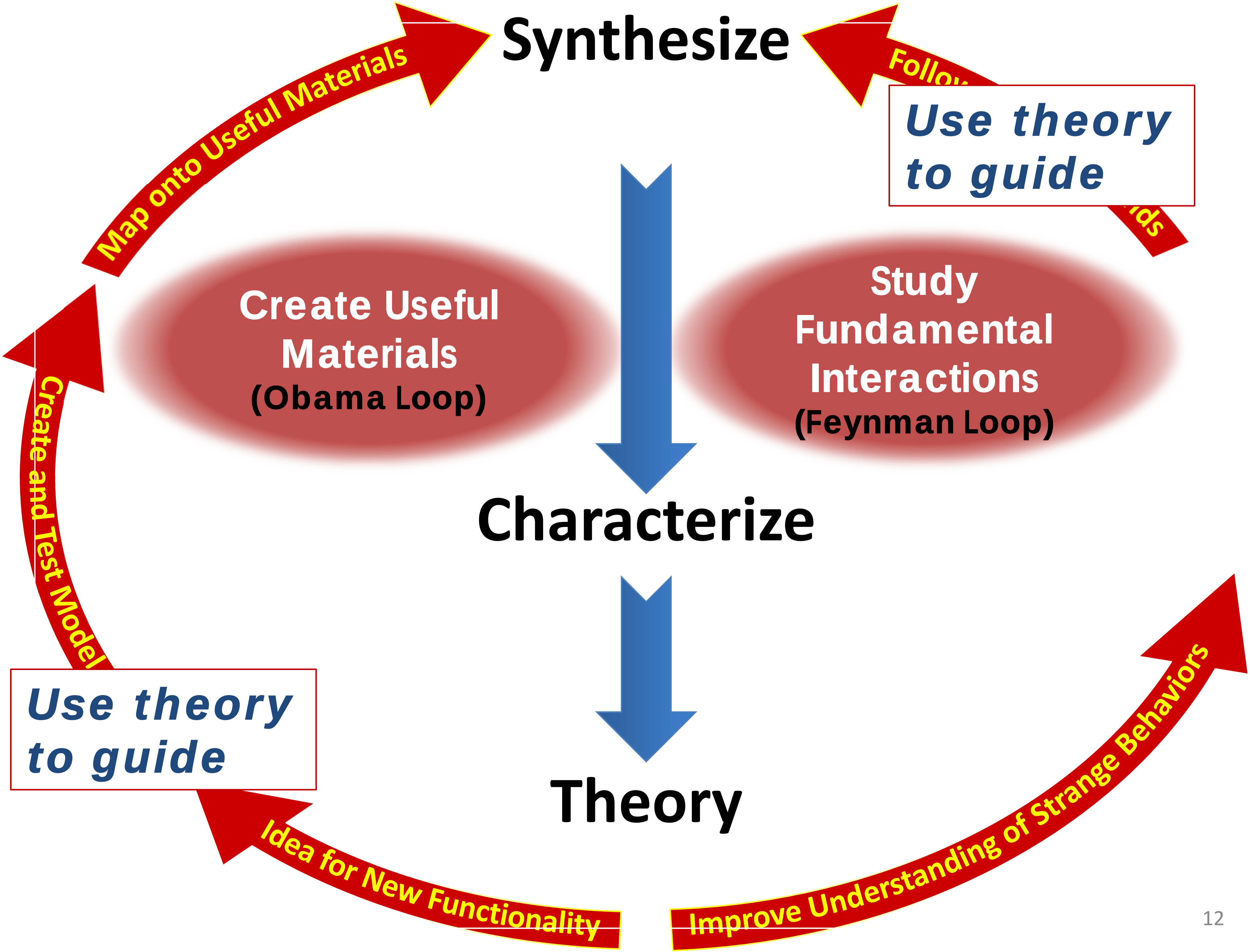
Perspective from the frontiers of complex oxide materials by design

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

"Rule 1": Fundamental science and applied science (engineering) do not belong together

"Rule 2": Theory and experiment are separate

"Rule 3": theoretical physicists and chemistry don't belong in engineering


Synthesize
Map onto Useful Materials
Use theory to guide
Create Useful Materials (Obama Loop)
Study Fundamental Interactions (Feynman Loop)
Characterize
Create and Test Model
Use theory to guide
Theory
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
- Whose main application focus so far has been in electronic and magnetic devices

Why these applications/materials: The stars have aligned at Cornell with a the majority of the faculty "pieces of the puzzle" for these applications joining at the same time

Advanced Materials

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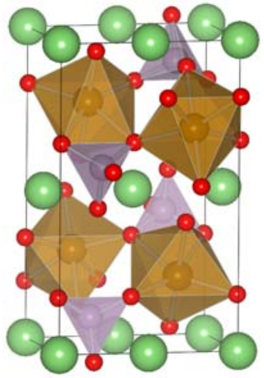
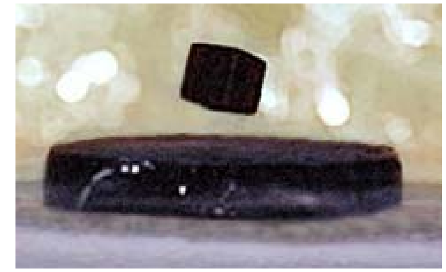
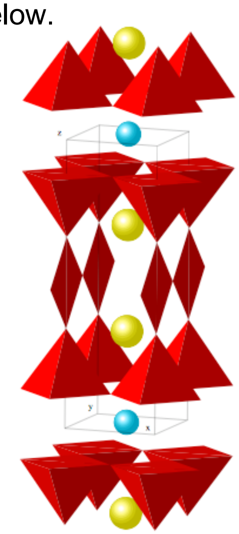
A High Resolution Transmission Electron Microscopy image of a $BaTiO_3/SrTiO_3$ superlattice grown by Molecular Beam Epitaxy [Schlom, et al. J. Am. Cer. Soc. **91** 2429 (2008)].
J. Heber, Nature **459** 28 (2009)



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.

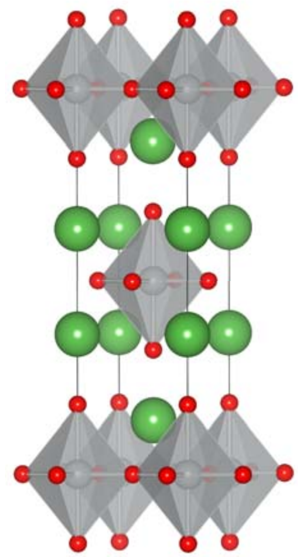


High-temperature superconductivity was first discovered in a layered oxide material. The structure of the superconductor $YBa_2Cu_3O_{7-\delta}$ is shown below.

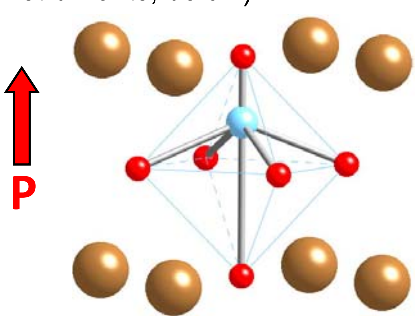


An Energy Server (manufactured by Bloom Energy), a power generator that uses Solid Oxide Fuel Cells.

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



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.

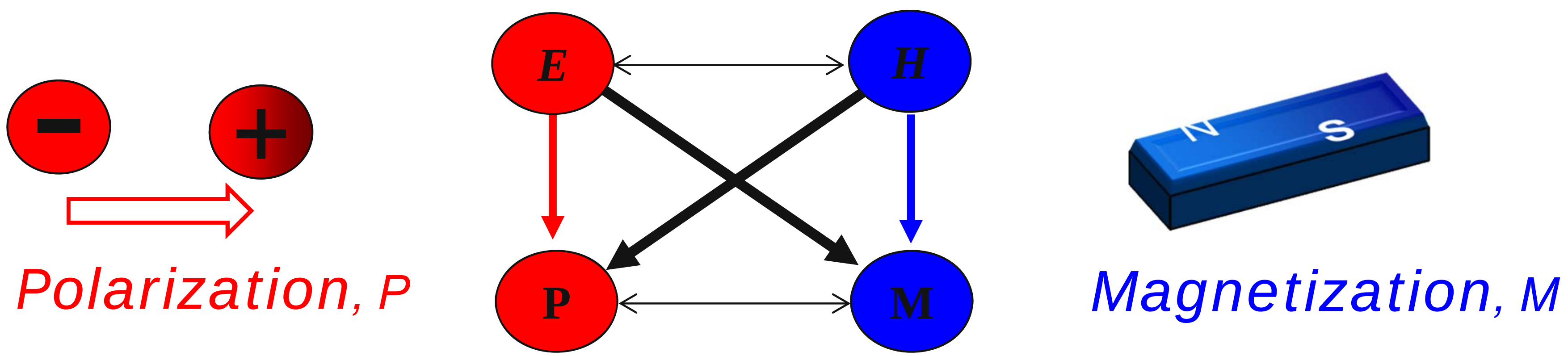


A ferroelectric distortion in the perovskite oxide $PbTiO_3$, one of the materials used in FeRAM devices. The arrow shows the direction of the electrical polarization.

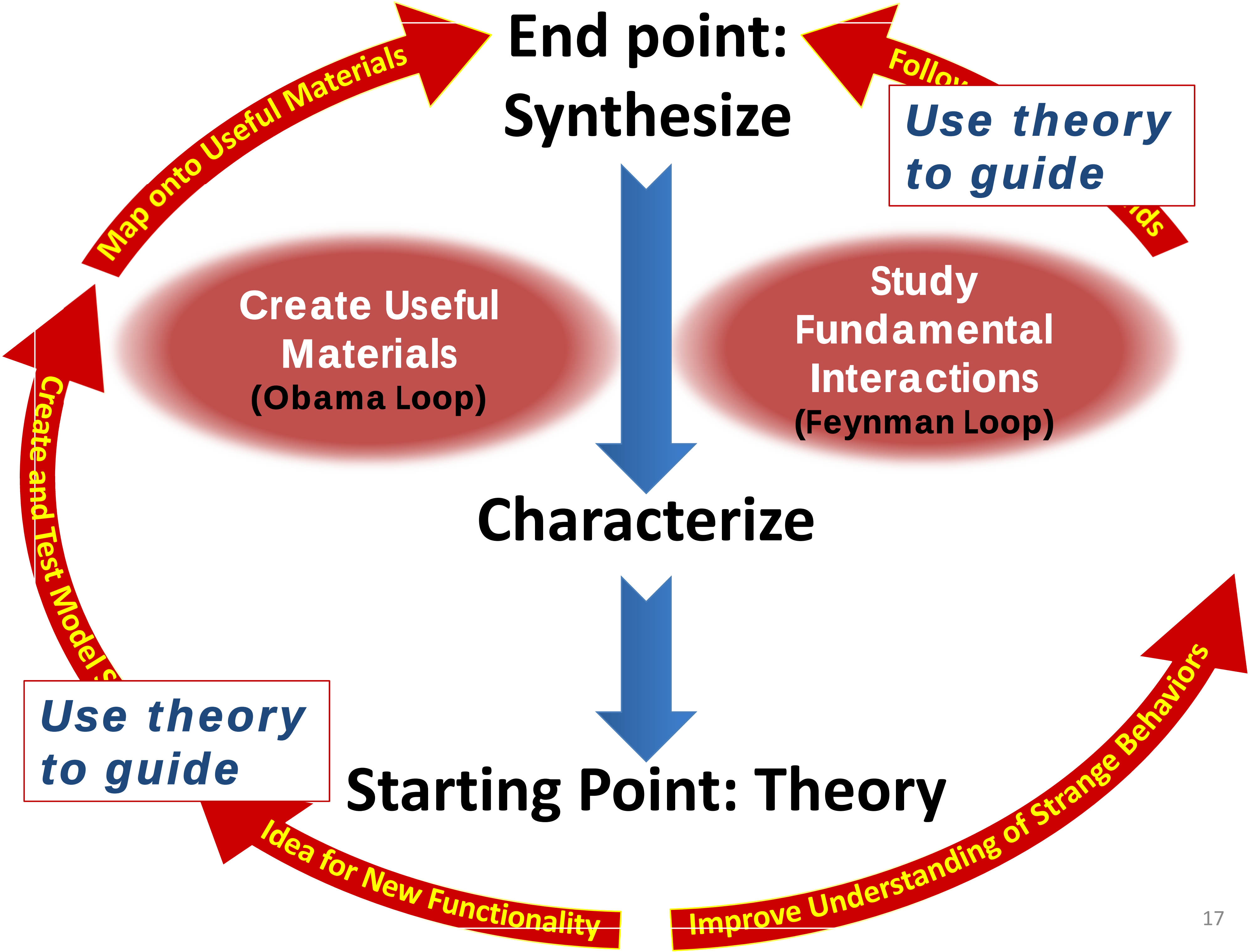
Oxides and oxide-like materials are important to many different areas of science and society, from fundamental science to electronic devices and clean energy technologies

An Example: Multifunctional magnetoelectrics

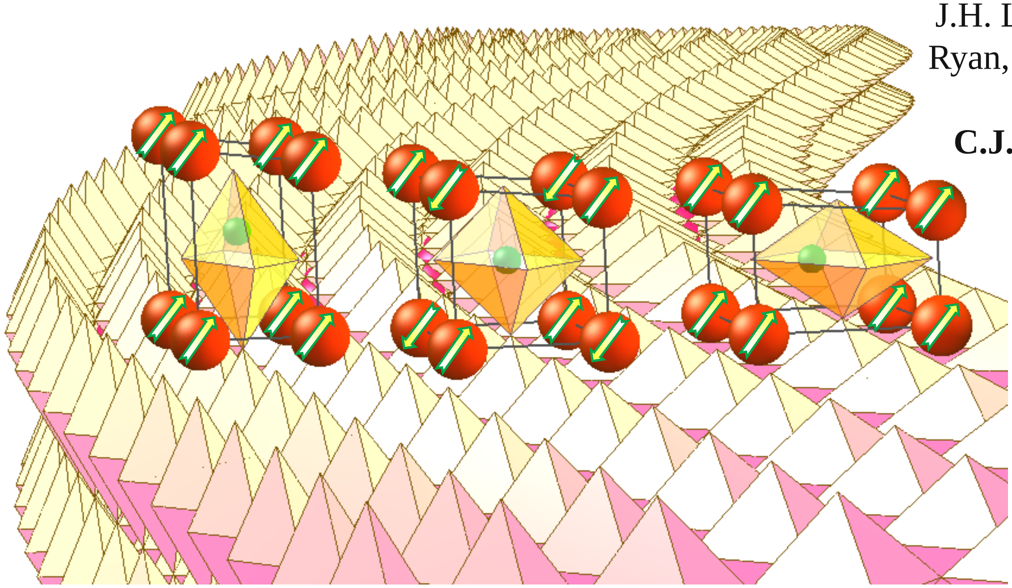
(Generalized) **Magnetoelectric**: cross coupled response to electric and magnetic fields



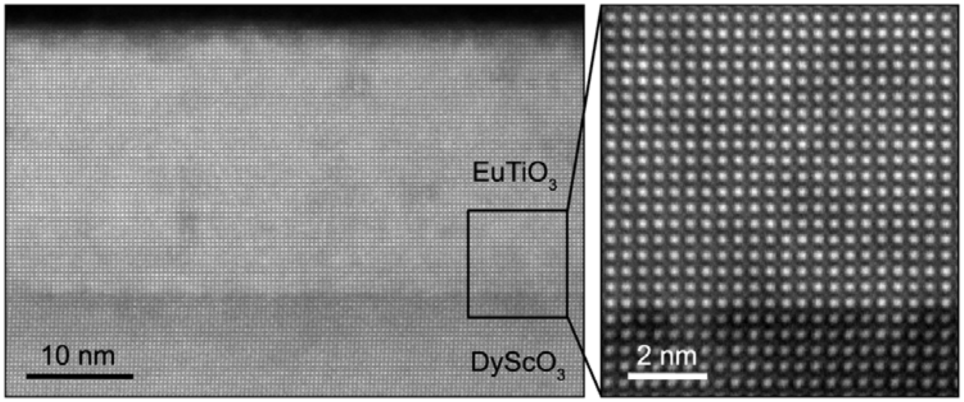
i.e. control of the magnetic **M** *(electric* **P***) phase with an applied electric* **E** *(magnetic* **H***) field*


End point: Synthesize
Characterize
Starting Point: Theory
Create Useful Materials
(Obama Loop)
Study Fundamental Interactions
(Feynman Loop)
Map onto Useful Materials
Create and Test Model S
Idea for New Functionality
Improve Understanding of Strange Behaviors
Use theory to guide
Use theory to guide

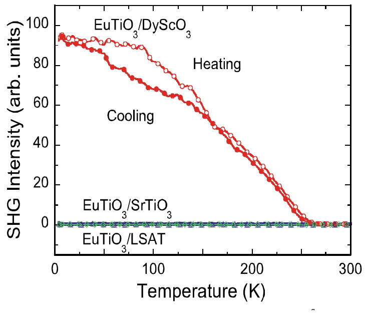
Strongest Ferromagnetic Ferroelectric



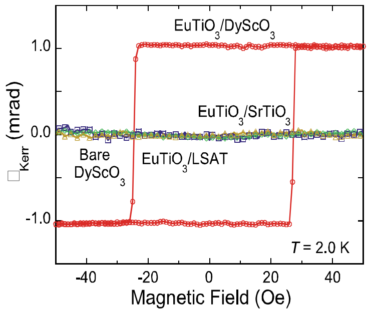
J.H. Lee, L. Fang, E. Vlahos, X. Ke, Y.W. Jung, **L.F. Kourkoutis**, J-W. Kim, P.J. Ryan, T. Heeg, M. Roeckerath,V. Goian, M. Bernhagen, R. Uecker, P.C. Hammel, K.M. Rabe, S. Kamba, J. Schubert, J.W. Freeland, **D.A. Muller**, **C.J. Fennie**, P. Schiffer, V. Gopalan, E. Johnston-Halperin, and **D.G.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

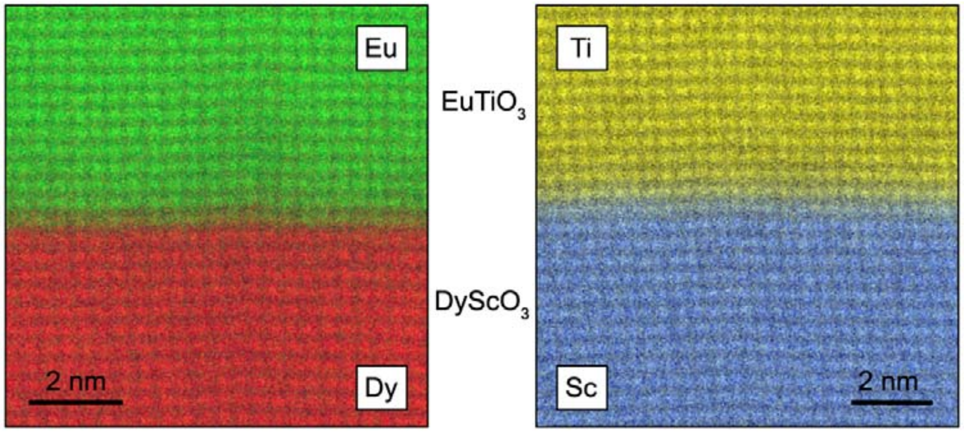


Ferroelectric
P ~ 20 µC/cm2



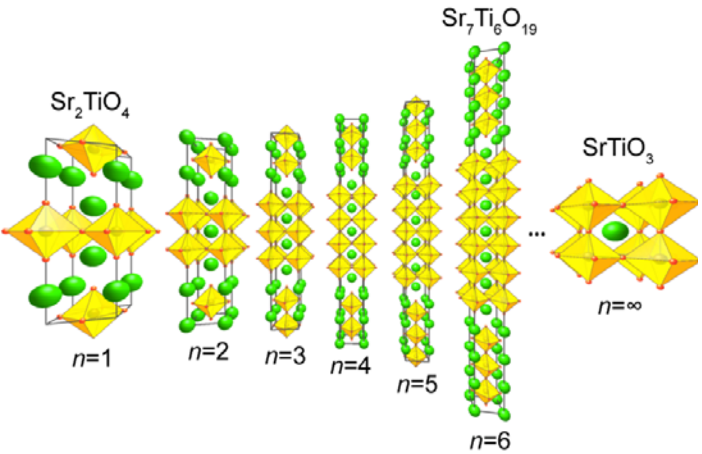
Ferromagnetic
~ 5 μ_B/Eu

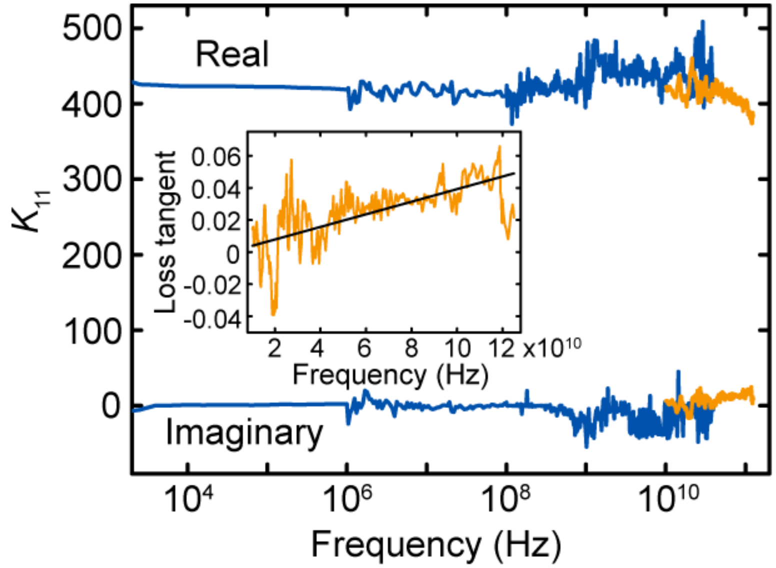


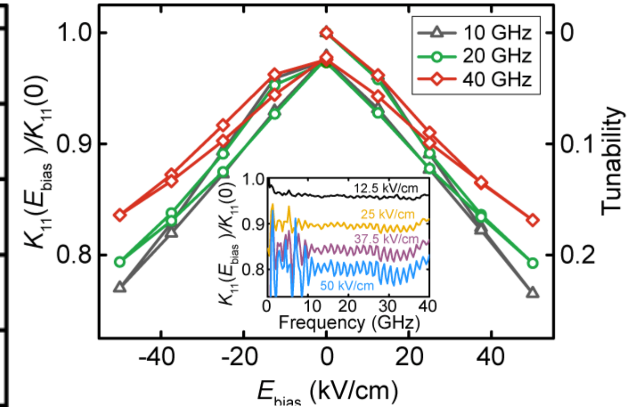


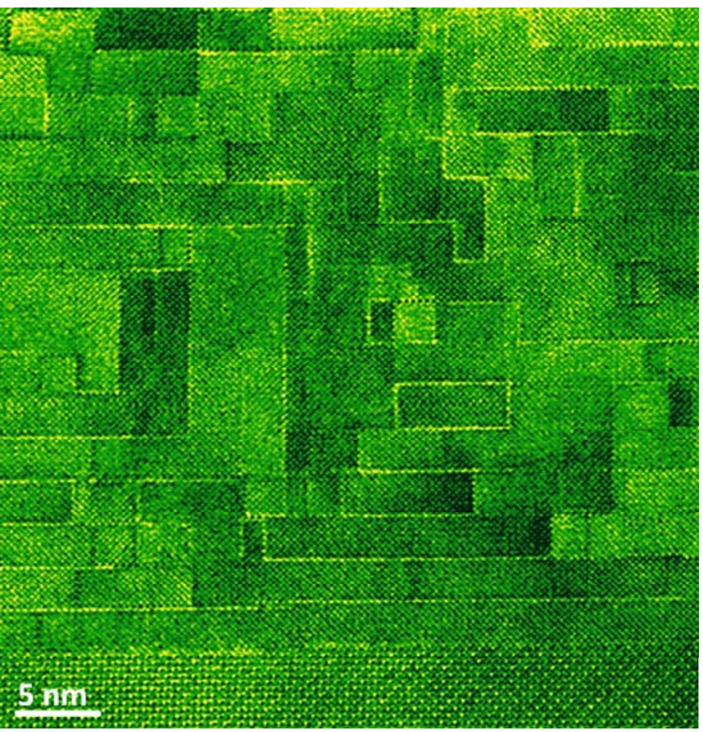
22 nm thick $EuTiO_3$ (a boring dielectric) + 1.1% Strain (by growing it commensurately) = Multiferroic (1000× stronger than prior ferromagnetic ferroelectrics)

Tunable Dielectric (GHz) with Performance 5-50× better than any Previously Known Material



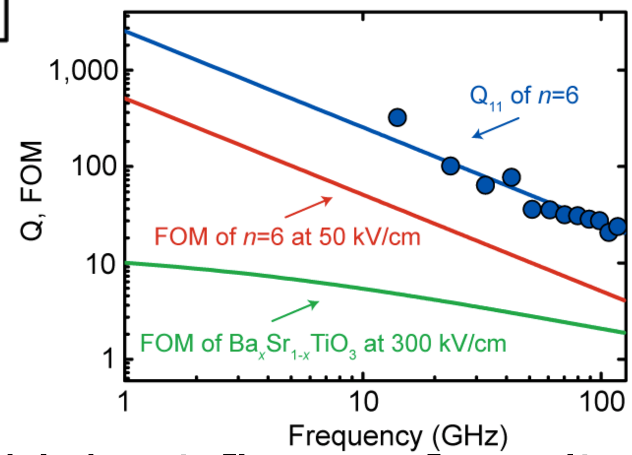






What's different?

Loss!



$Sr_7Ti_6O_{19}$ (n = 6) has highest figure of merit (FOM) of any known tunable dielectric

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.

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)
- MBE + ARPES

Why Cornell !: Our approach to materials discovery requires …

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

Students trained in physics, chemistry, and materials science

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

Even at Cornell, which has no boundaries between departments, this can be difficult because of established culture within disciplines (I have ideas …)

The implementation of Erza's vision …

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Phase I—Moore Foundation

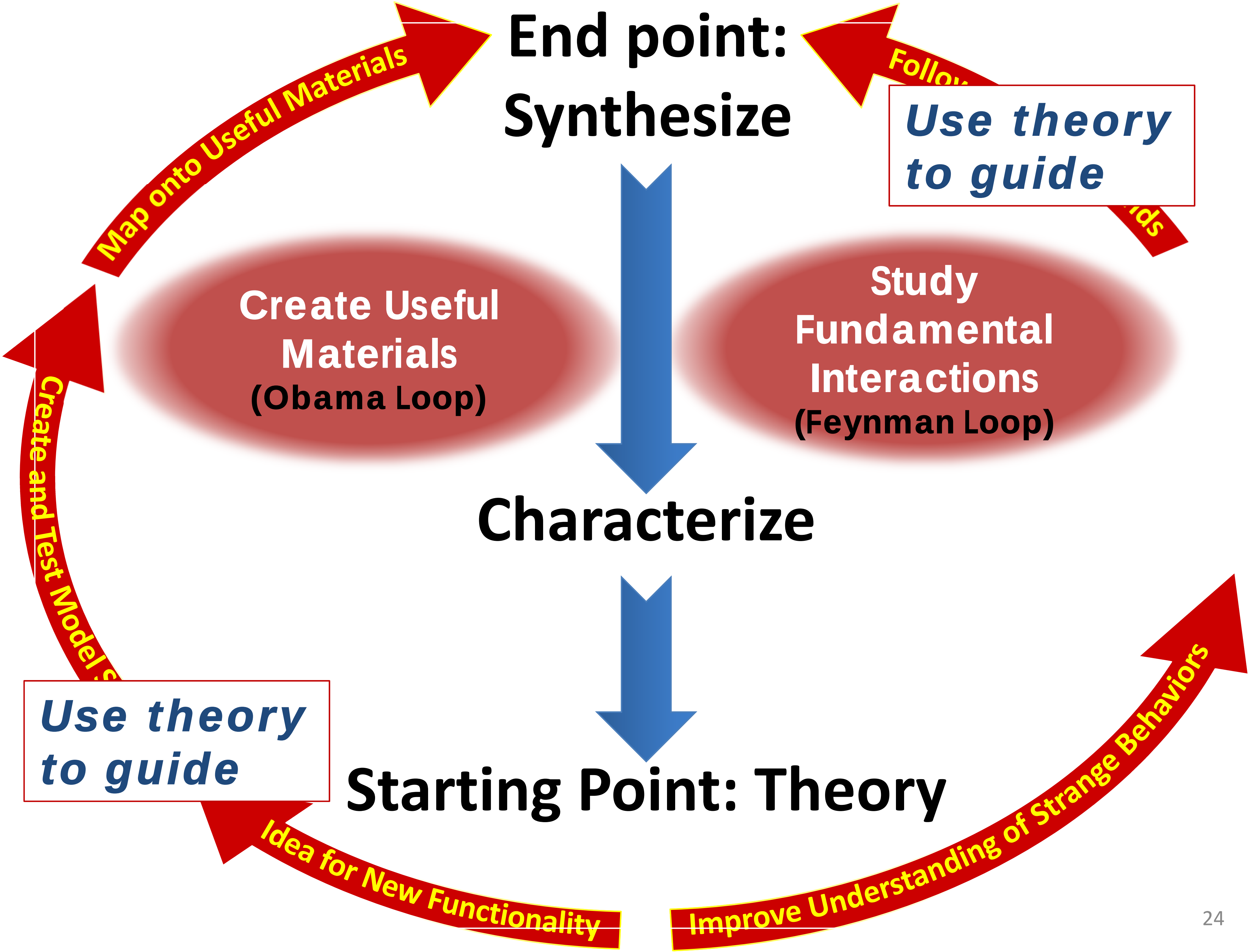
Emergent Phenomena in Quantum Systems (EPiQS)

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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Synthesize
Use theory
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Map onto Useful Materials
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Materials
(Obama Loop)
Study
Fundamental
Interactions
(Feynman Loop)
Characterize
Create and Test Model
Use theory
to guide
Starting Point: Theory
Idea for New Functionality
Improve Understanding of Strange Behaviors

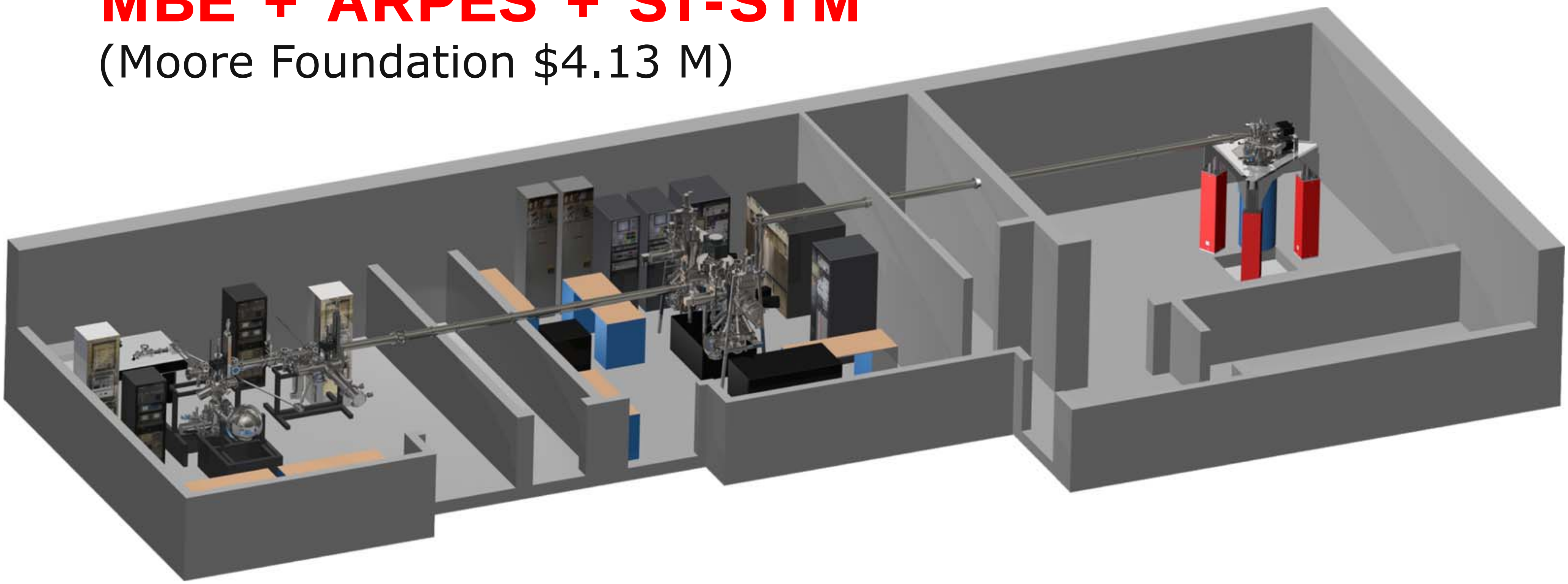
Moore money: Instrumentation development

Emergent Phenomena in Quantum Systems (EPiQS)

The first (and only)

MBE + ARPES + SI-STM

(Moore Foundation $4.13 M)



Moore money: 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 …

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

Phase II—NSF

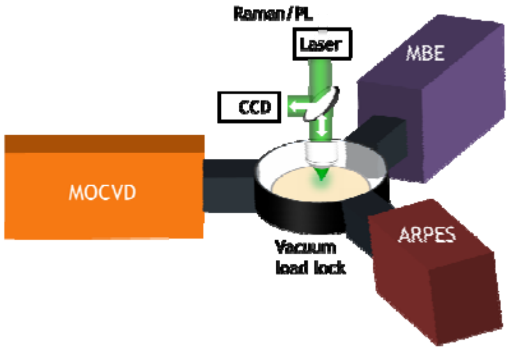
Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM)

- $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)

<u>In-House Research Program</u>

Creating Interface Materials with Designed Properties



ACTIVE SUBSTRATE + THIN FILM

New Chemistry
New Physics
New Materials Science

<u>User Facility</u>

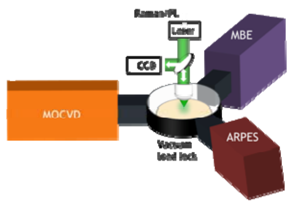
Accelerating the pace at which new bulk and thin film crystalline materials are designed, realized experimentally, and measured

CASCADE

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

Creating Interface Materials with Designed Properties

+



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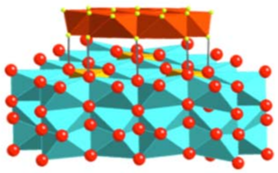
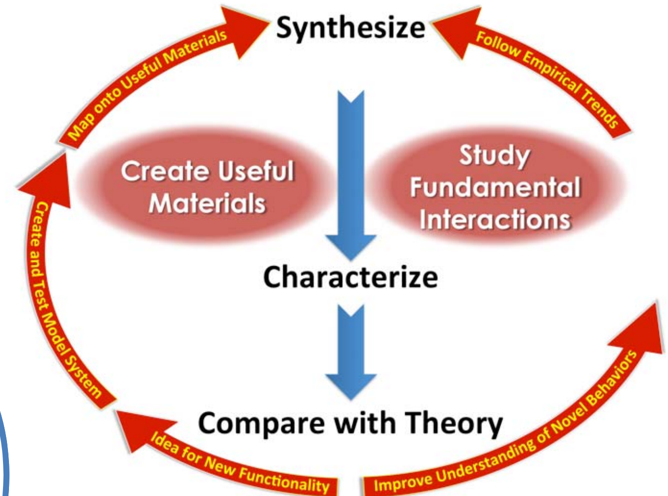
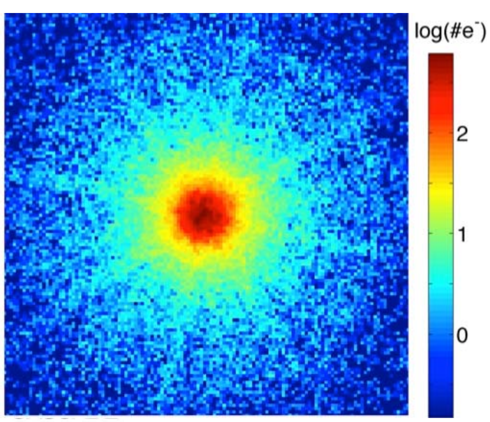


Empowering Users



CASCADE

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

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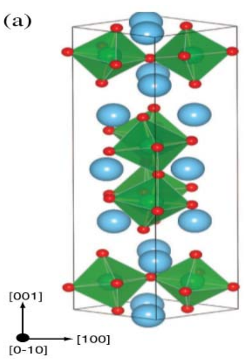
Next Steps: Theory Postdoctoral center

Moore and the NSF made a gigantic investment in the 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 should seed a Theory Postdoctoral related to CASCADE (administered by the Cornell Kavli Center: I've been told that Kavli will match the contribution) for two reasons
  - 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

Need (faculty in) bulk single crystal scientist

New *bulk* materials by design



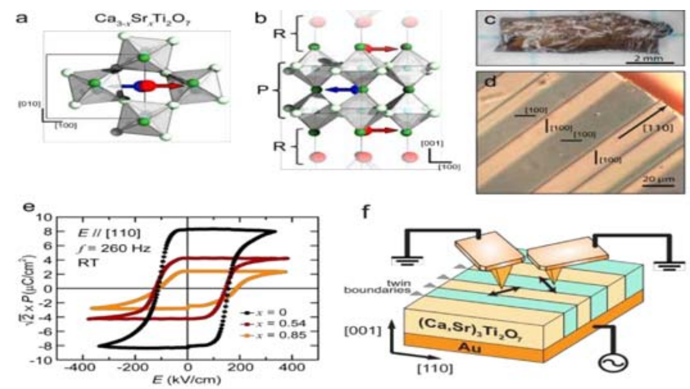
Theoretical discovery

- A new "kind" of ferroelectric
  Benedek and Fennie, Phys. Rev. Lett 2011
- New crystal-chemistry
  Fennie and coworkers 2012-2013
  (Adv Mat, Adv Func. Mat.)

Experimental confirmation

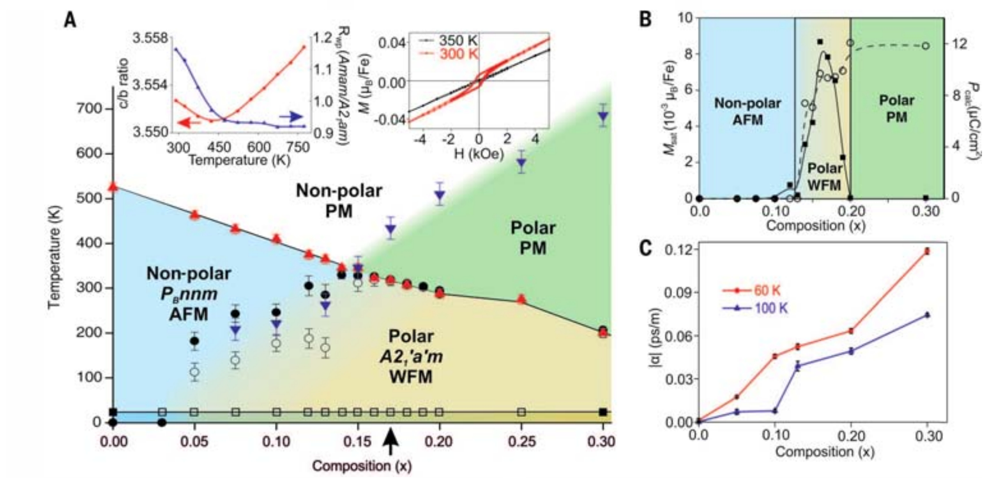
(bulk single crystals) S-W Cheong, Rutgers

2015 Nature Materials

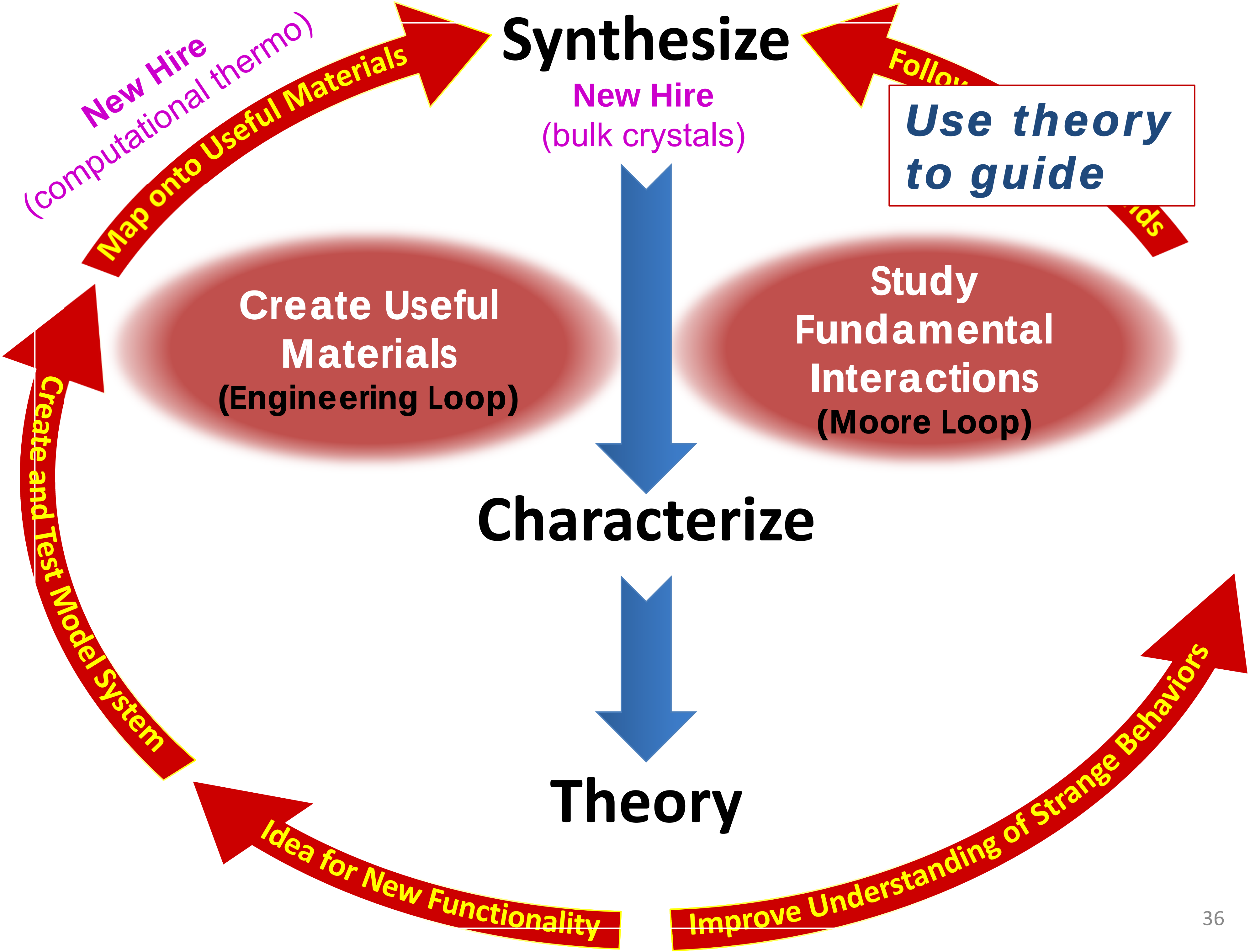


Experimental confirmation

(bulk) M Rosensky, Liverpool
2015 Science



2015 (Science)
Hybrid Improper ferroelectricity experimentally demonstrated to induce linear magnetoelectricity, as predicted by Fennie, in a bulk RP material system.


Synthesize
New Hire
(bulk crystals)
New Hire
(computational thermo)
Map onto Useful Materials
Use theory to guide
Create Useful Materials
(Engineering Loop)
Study Fundamental Interactions
(Moore Loop)
Characterize
Create and Test Model System
Theory
Idea for New Functionality
Improve Understanding of Strange Behaviors

Next Steps

- Initiate Faculty Search to Fill 2 Gaps
  - Solid State Synthesis
  - Computational Thermodynamics
- Possible Solid State Synthesis Expert (in A&S?)
- Possible Computational Thermo—Cornell Engineering
- Hire expert in new application, e.g., photovoltaics, to help take our approach in a new direction

New Bold Directions to be Added