FOUR REQUESTS from an Experimentalist to bold Theorists

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My Four Requests

- Please do *not* Pollute the Literature with Predictions on Impossible Materials

Literature protocol:

Assume hypothetical structure, then predict (e.g, via DFT) an interesting properties.

But does the assumed structure have a chance to exist ?

Prof. Alex Zunger
University of Colorado
Alex.zunger@colorado.edu

Exciting properties of impossible material

- **Optoelectronic** properties of 120 hypothetical ABX compounds (e.g. KCaN) were evaluated (literature) in assumed structures .We found (via DFT) most of these compounds would phase-separate into binaries.

- **Topolgical insulating** properties were predicted for LiHgAs, LiHgSb, NaHgAs etc (literature) . We found these structures are thermodynamically unstable w.r.t. decomposition into binaries

Fermion quasiparticle in the SiO_2- structure-type of BiO_2.

- **Harder-than-diamond** cubic C_3N_4 proposed in literature (actually it is dynamically unstable in this crystal structure)

Global Space-Group Optimization (GSGO)

(Trimarchi & Zunger 2007 Phys Rev B)

Randomly generated structures

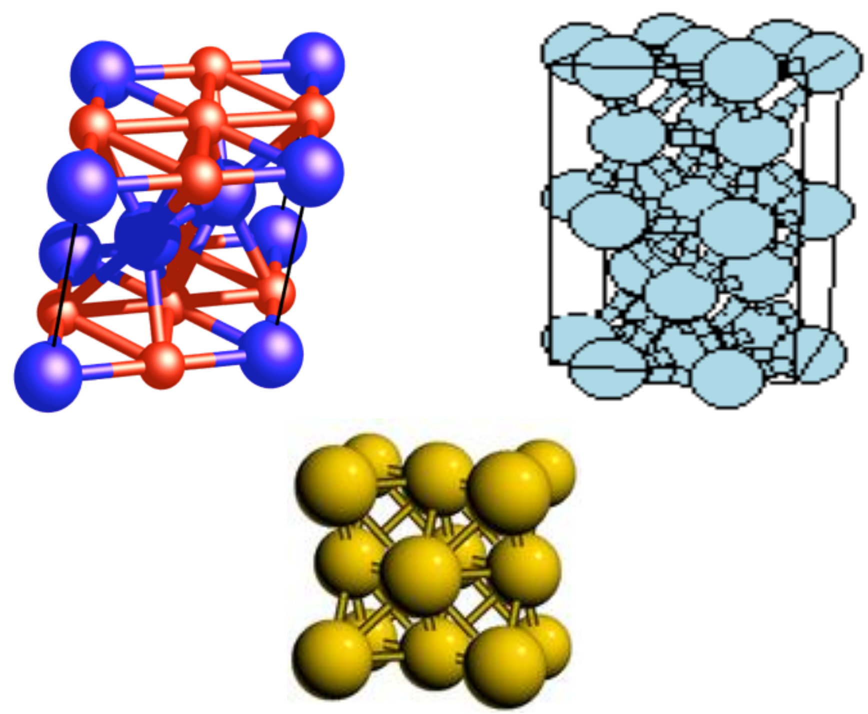
Parental population

Generate off-springs via real -space crossover and mutation

Calculation of the fitness function (free energy)

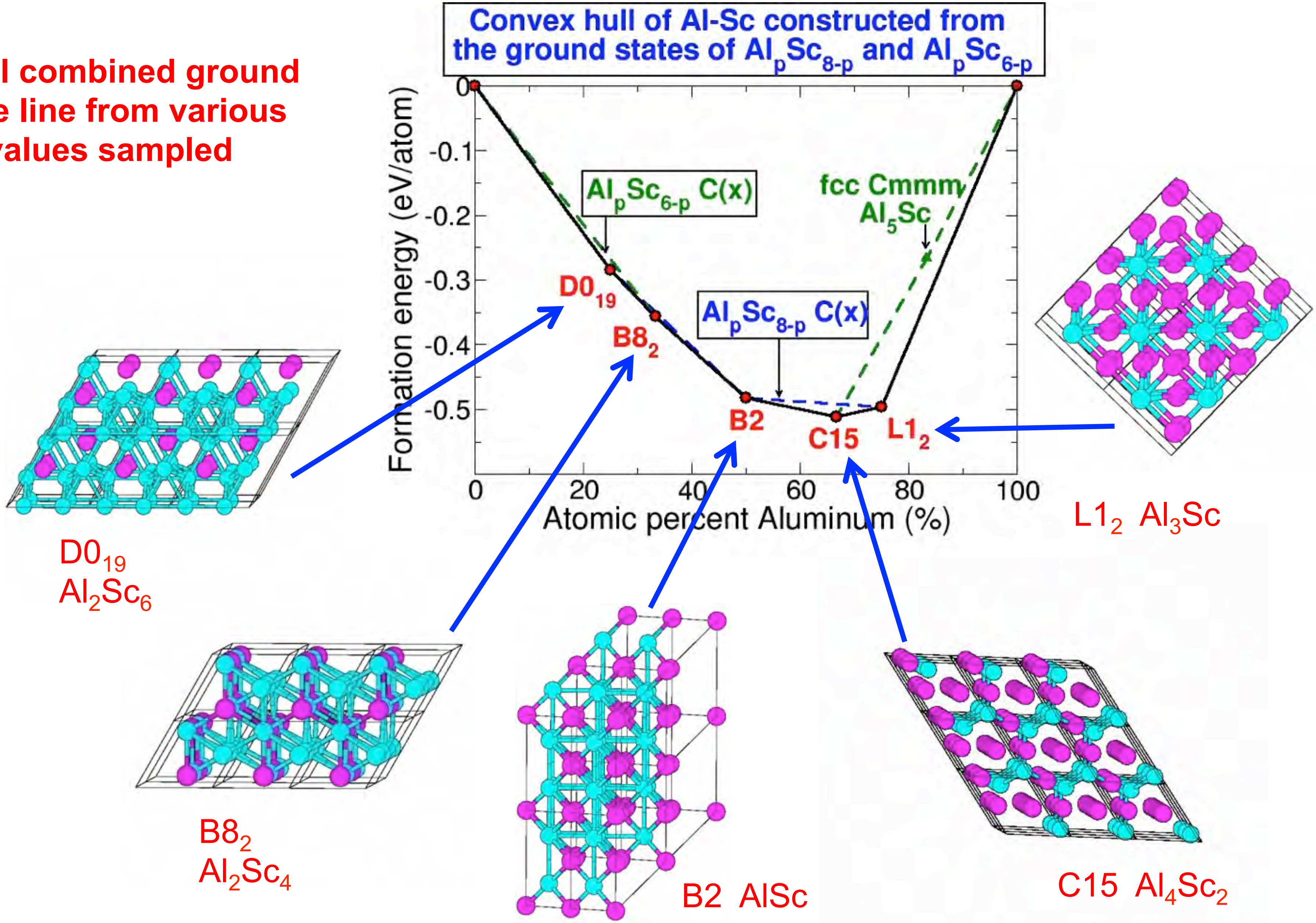
Selection

Produce initial random generation, which becomes the parental population

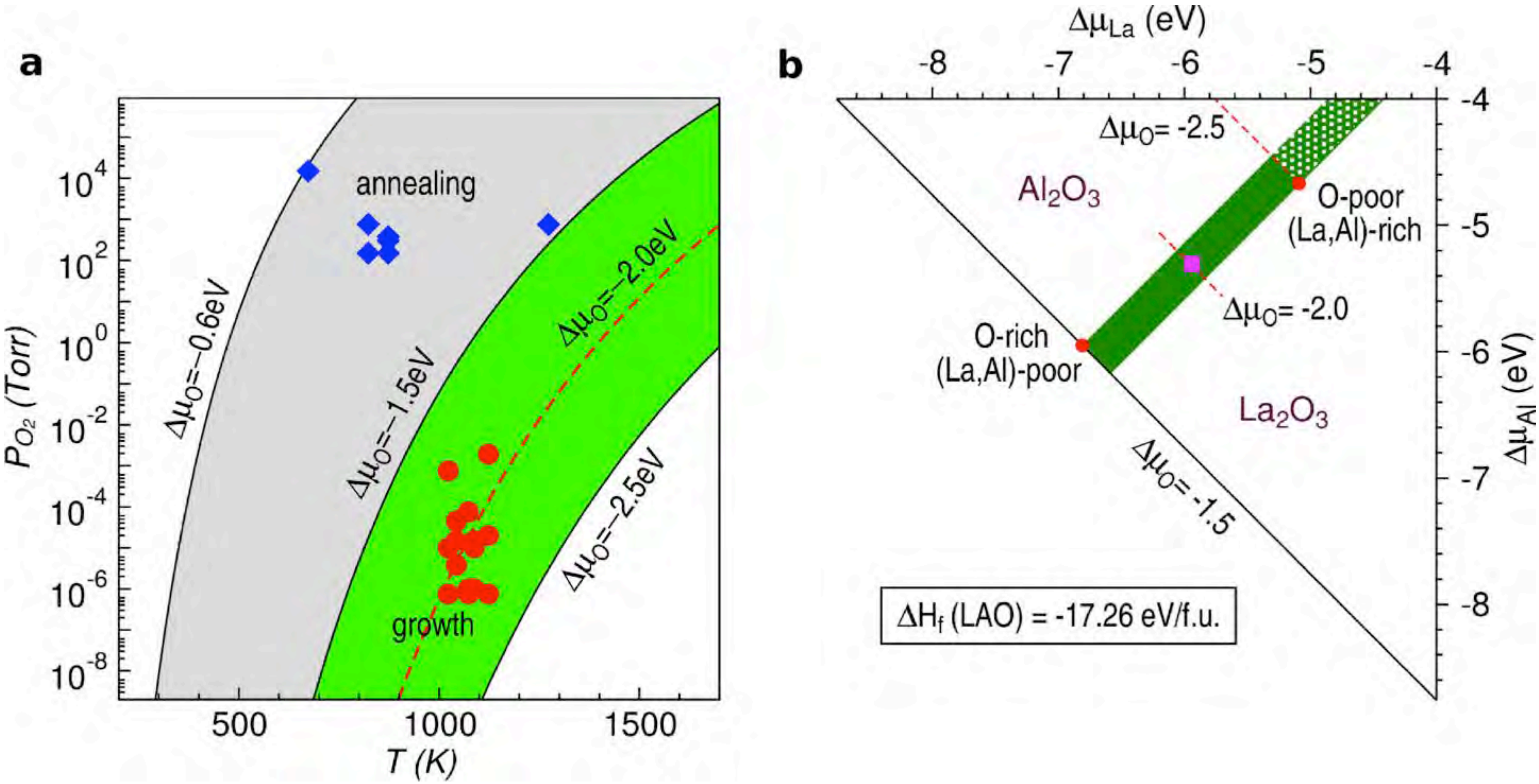


Example of X-GSGO

Final combined ground state line from various N_{at} values sampled



Growth conditions



My Four Requests

- Please do *not* Pollute the Literature with Predictions on Impossible Materials

- Please *do* Consider the Limits of Synthesis

Important Synthesis Rules

- **Gibbs' Rule**
  $\Delta G < 0$ to form stable phases
- **Matthias's Rules for Superconductors**
  … "Stay away from Theorists"
- **Pauling's Rules for Crystal Structures**
  Radius ratio criteria for stability

Rules for QM Synthesis

- Gibbs' Rule
  $\Delta G < 0$ to form stable phases
- Matthias's Rules for Superconductors
  … "Stay away from Theorists"
- Pauling's Rules for Crystal Structures
  Radius ratio criteria for stability

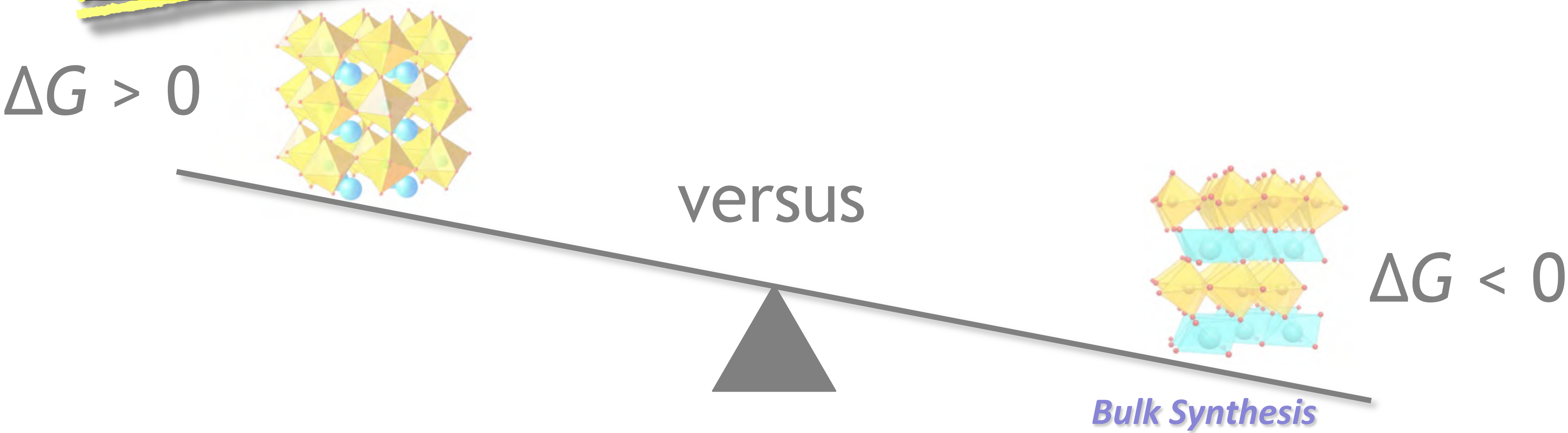
BREAK THE RULES!

BREAK THE RULES

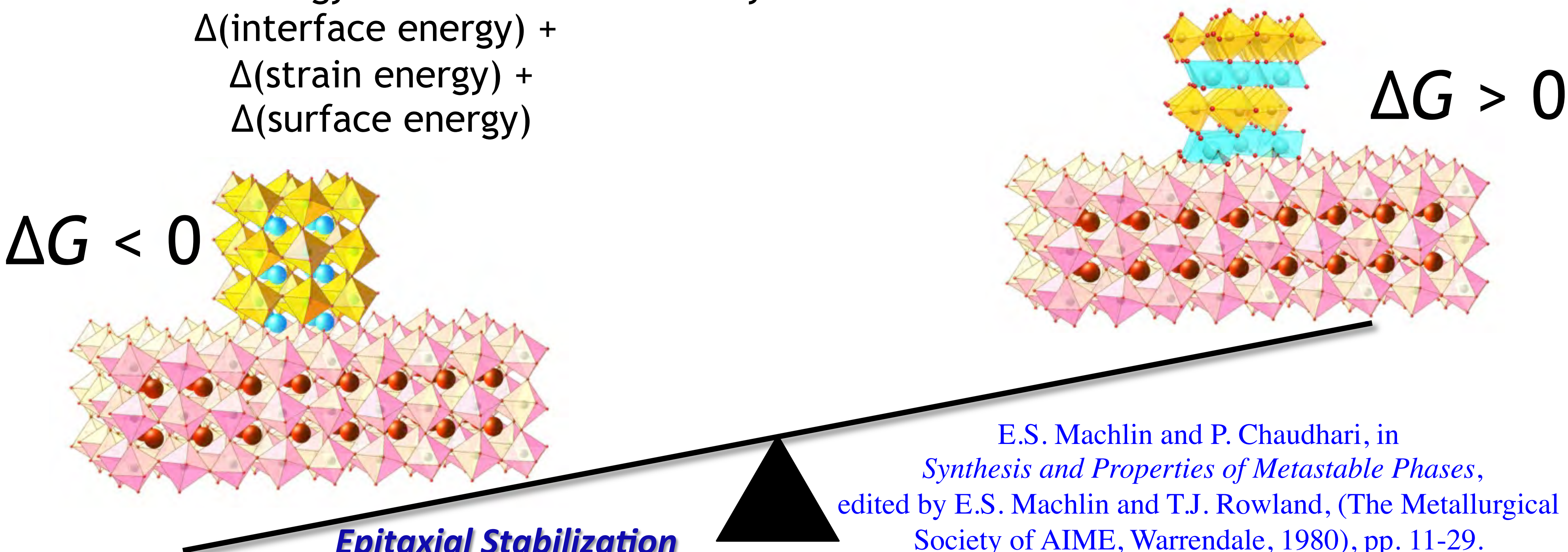
- Gibbs' Rule

  $\Delta G < 0$ to form stable phases

BREAK Gibbs' Rule



Stable if free energy difference overcome by
Δ(interface energy) +
Δ(strain energy) +
Δ(surface energy)



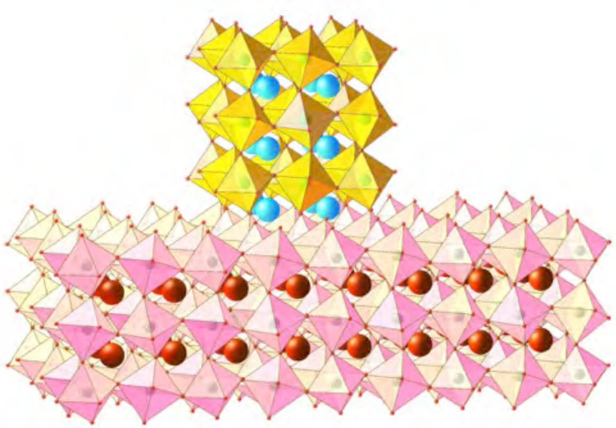
E.S. Machlin and P. Chaudhari, in *Synthesis and Properties of Metastable Phases*, edited by E.S. Machlin and T.J. Rowland, (The Metallurgical Society of AIME, Warrendale, 1980), pp. 11-29.

BREAK THE RULES

- Gibbs' Rule
  $\Delta G < 0$ to form stable phases
  Exploit interfacial energy from substrate

Substrates are Important

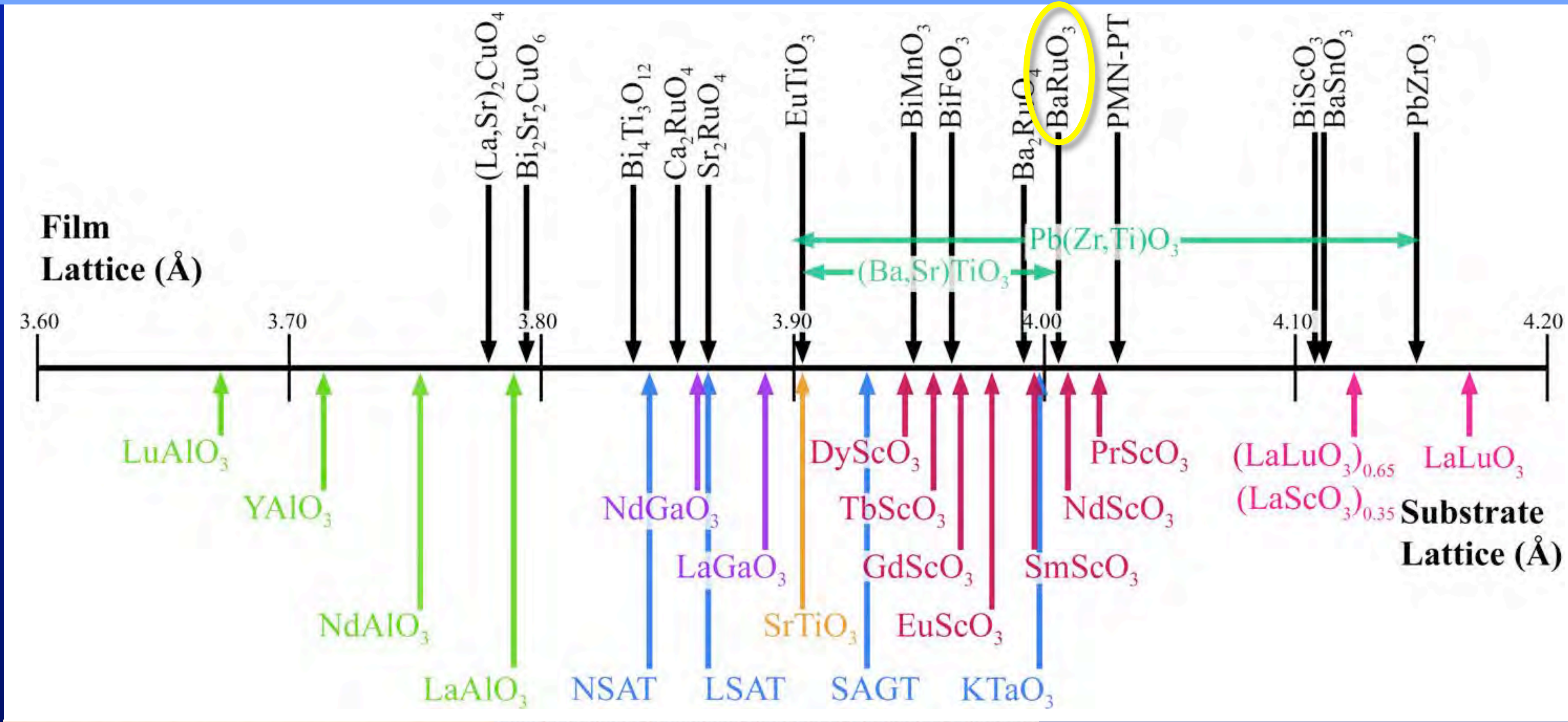
"Indeed, to achieve the objective of 'psuedomorphic stabilization,' the researcher should make the attempt to choose the substrate …"

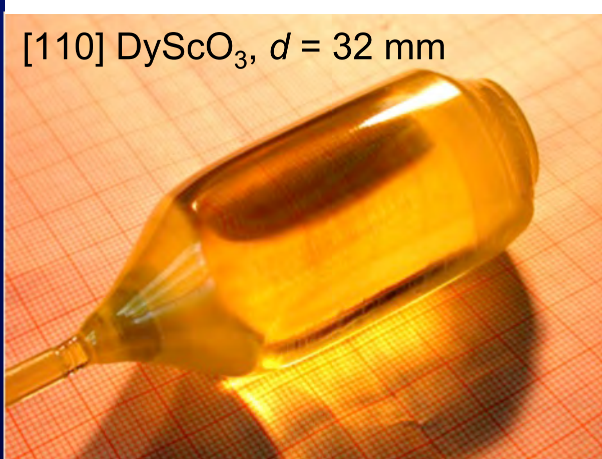


Epitaxial Stabilization

E.S. Machlin and P. Chaudhari,
"Theory of 'Pseudomorphic Stabilization' of Metastable Phases in Thin Film Form," in *Synthesis and Properties of Metastable Phases*, edited by E.S. Machlin and T.J. Rowland (The Metallurgical Society of AIME, Warrendale, 1980), pp. 11-29.

Commercial Perovskite Substrates

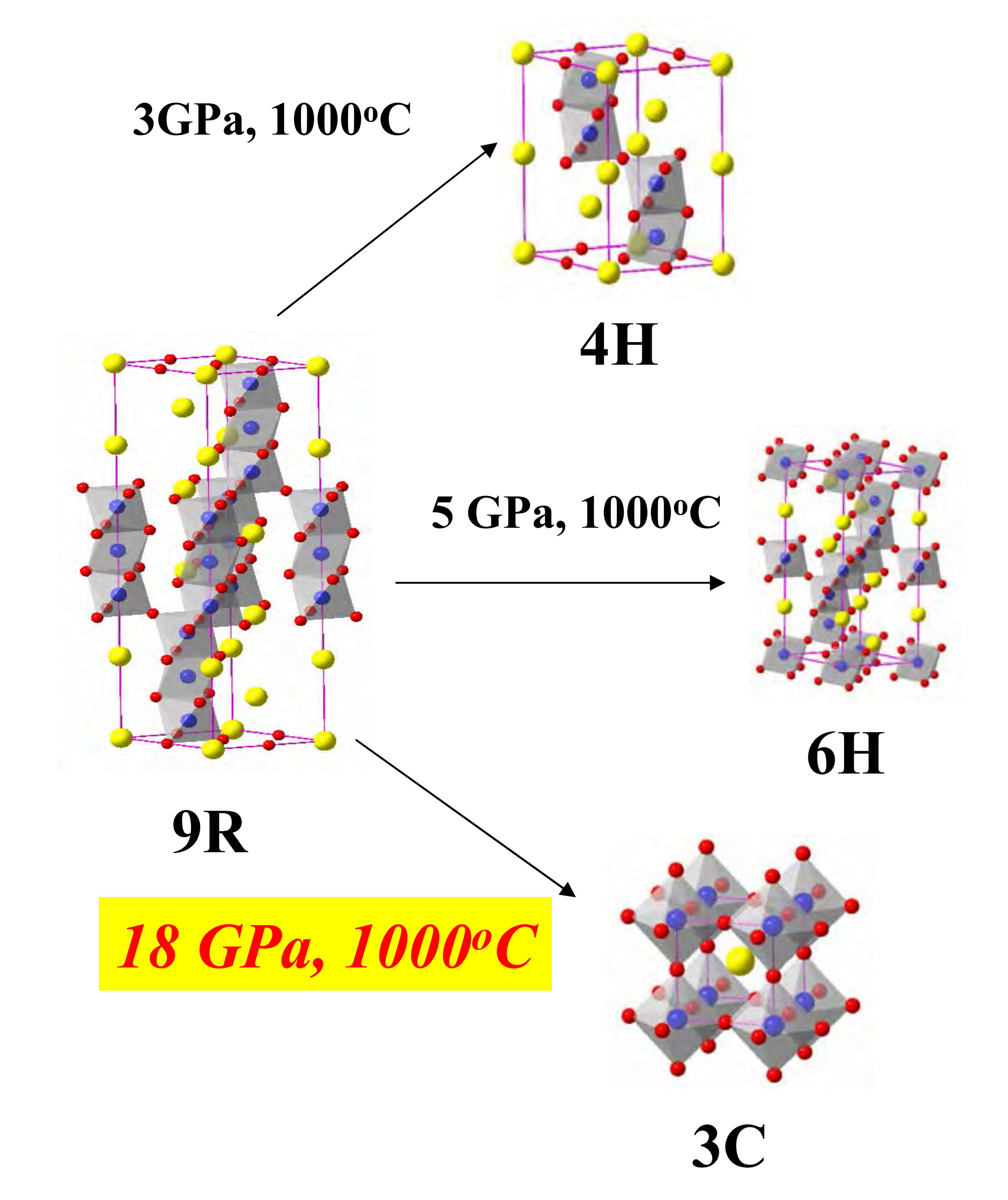


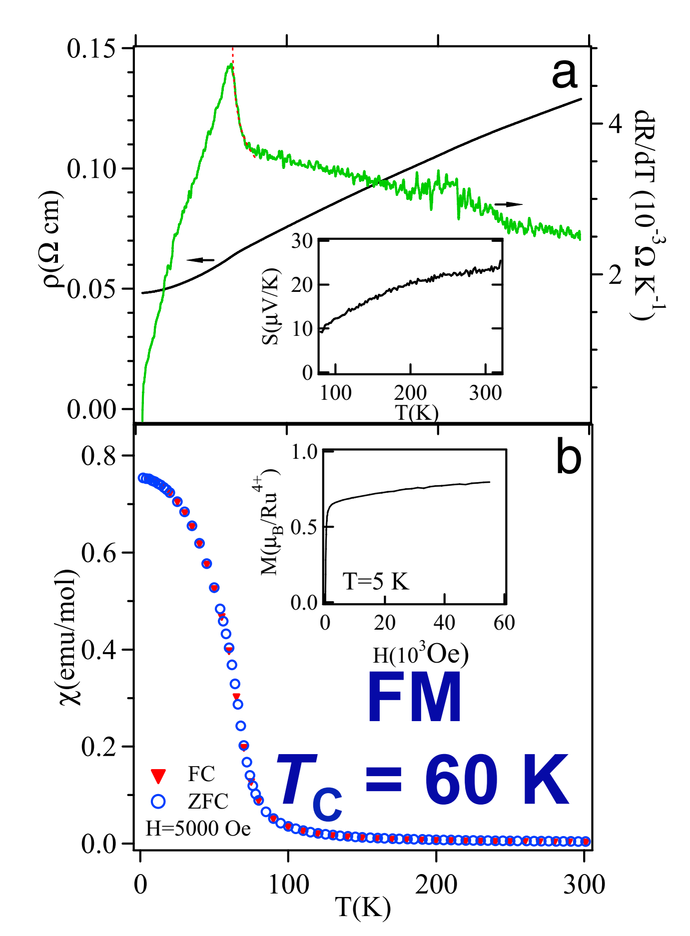

[110] DyScO$_3$, d = 32 mm


[110] GdScO$_3$, d = 32 mm

D.G. Schlom, L.Q. Chen, C.J. Fennie, V. Gopalan, D.A. Muller, X.Q. Pan, R. Ramesh, and R. Uecker, “Elastic Strain Engineering of Ferroic Oxides,” *MRS Bulletin* **39** (2014) 118-130.

$BaRuO_3$ Polymorphs

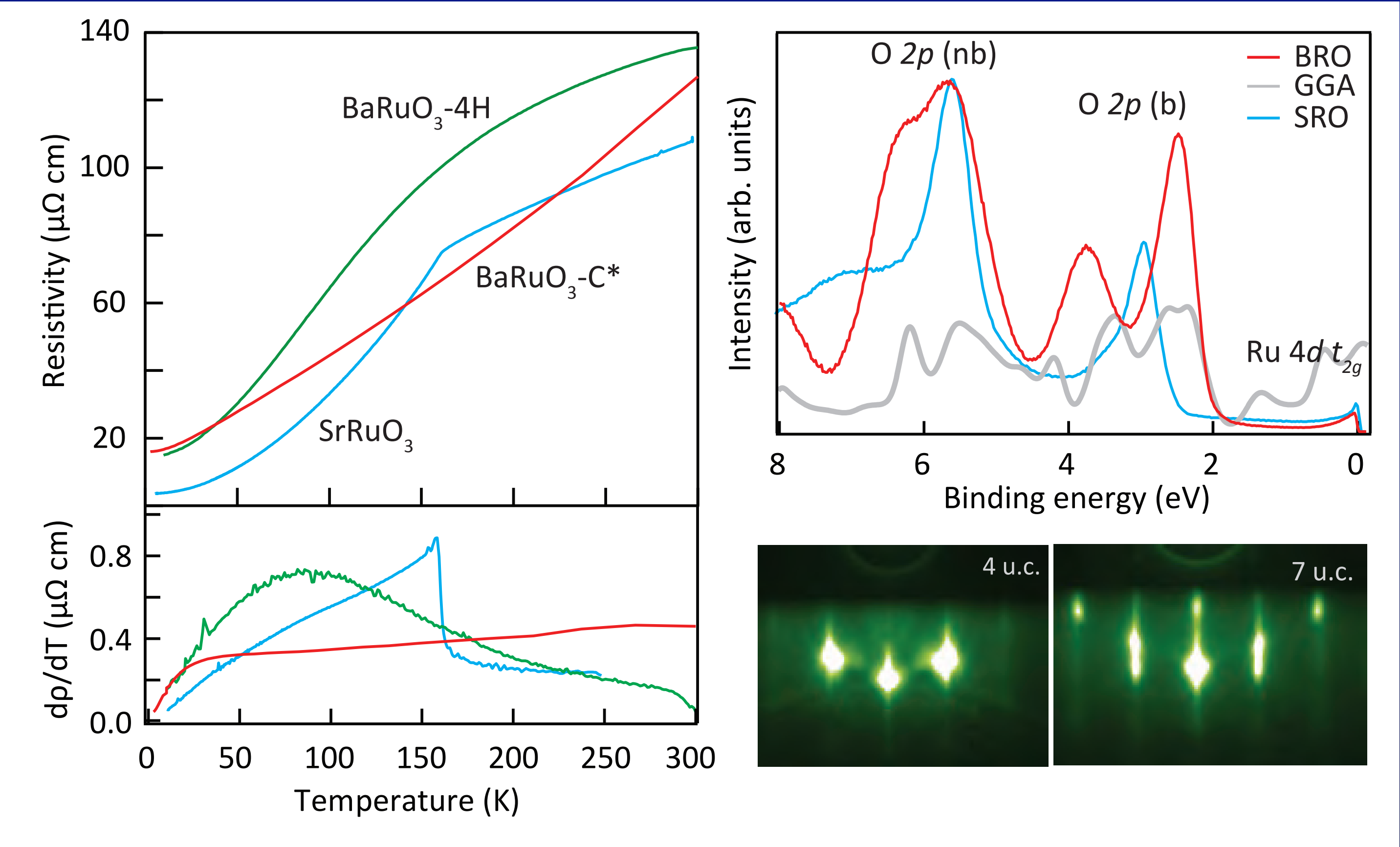




C.Q. Jin, J.S. Zhou, J.B. Goodenough, Q.Q. Liu, J.G. Zhao, L.X. Yang, Y. Yu, R.C. Yu, T. Katsura, A. Shatskiy, and E. Ito, "High-Pressure Synthesis of the Cubic Perovskite $BaRuO_3$ and Evolution of Ferromagnetism in $ARuO_3$ (A = Ca, Sr, Ba) Ruthenates," *PNAS* **105** (2008) 7115–7119.

Example — $BaRuO_3$ / $SrTiO_3$

- Epitaxially stabilized for ≤ 5 unit cells
- No octahedral rotations (2.5% compressive strain → tetragonal)
- $\frac{\rho_{300\ K}}{\rho_{4\ K}} = 7$
- No FM



BREAK THE RULES

- Gibbs' Rule
  $\Delta G < 0$ to form stable phases
  Exploit interfacial energy from substrate

- Matthias's Rules for Superconductors
  … "Stay away from Theorists"

Rules of B. Matthias for discovering new superconductors

1. high symmetry is best
2. peaks in density of states are good
3. stay away from oxygen
4. stay away from magnetism
5. stay away from insulators
6. stay away from theorists

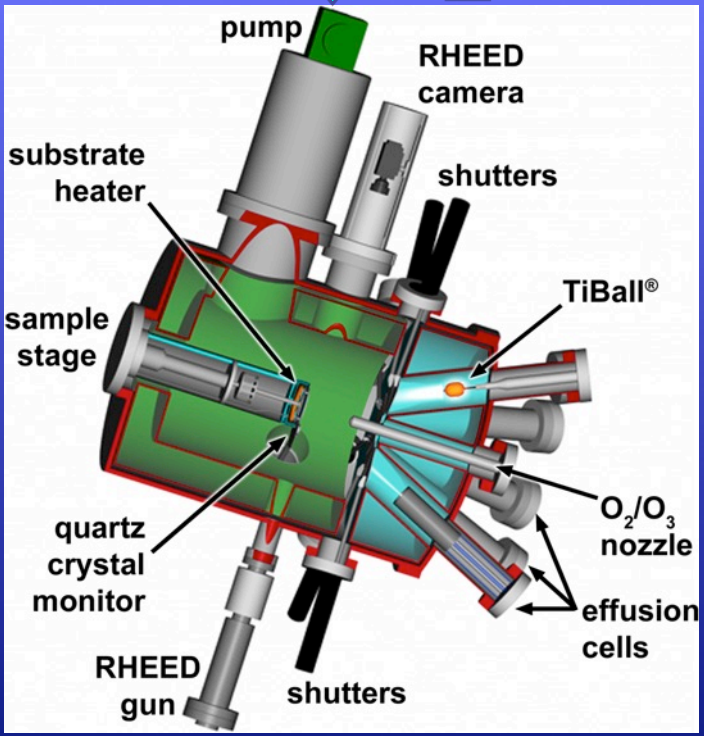
Scanned at the American Institute of Physics

From Steve Girvin's lecture (Boulder Summer School 2000) courtesy of Mike Norman via Matthew Fisher

BREAK

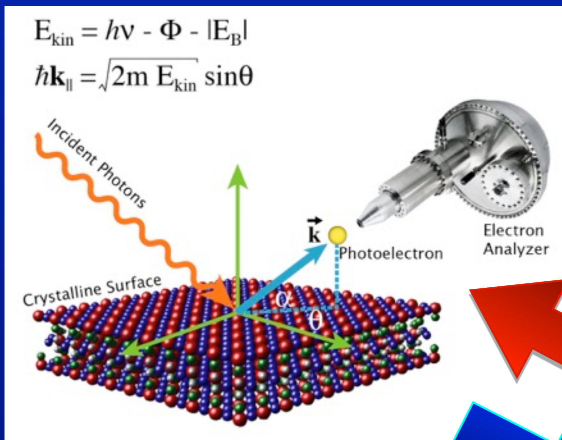
Matthias' Rule

Team up with Theorists

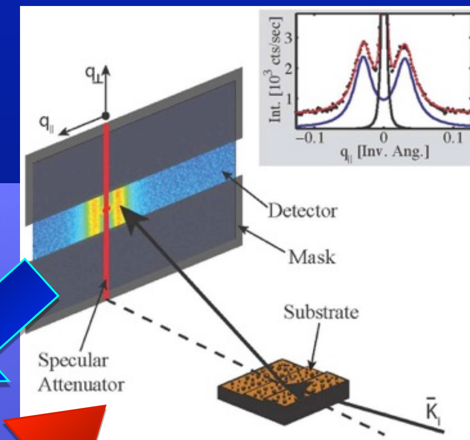


Thin-Film Synthesis

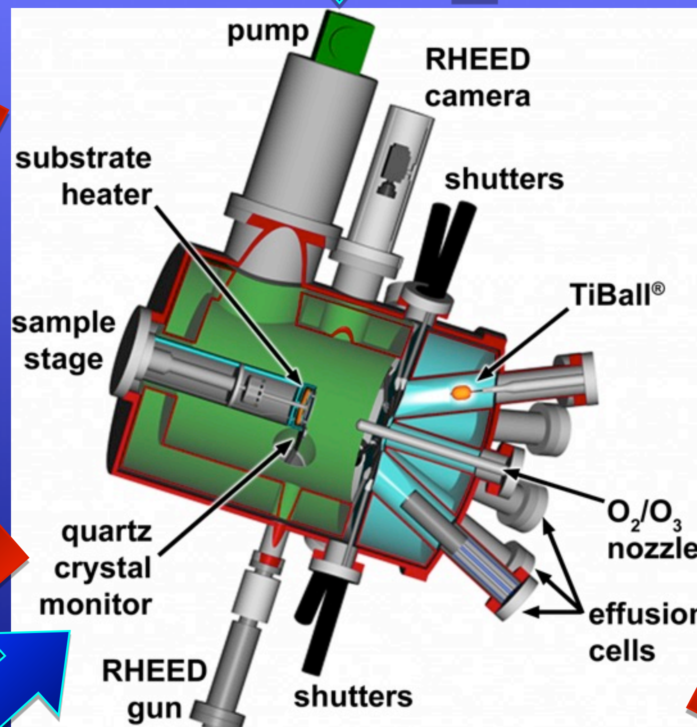
Provide useful Feedback to Theory



Theory

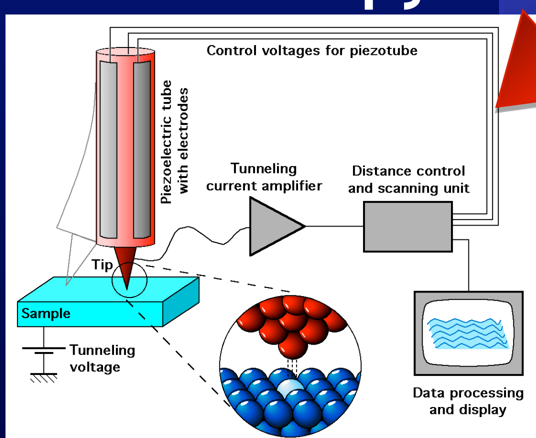


Photoemission Spectroscopy

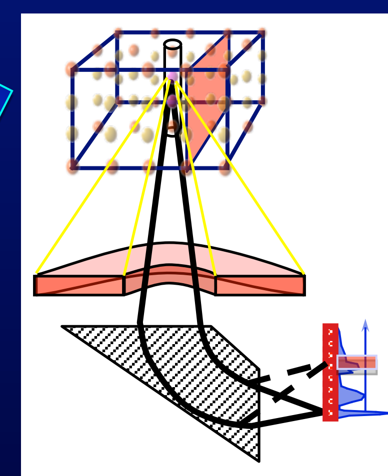


Synchrotron X-ray Diffraction

Scanning Tunneling Microscopy



Thin-Film Synthesis



Transmission Electron Microscopy

BREAK THE RULES

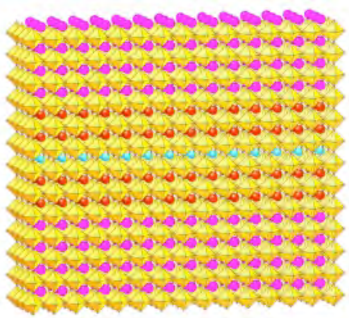
- Gibbs' Rule
  $\Delta G < 0$ to form stable phases
  Exploit interfacial energy from substrate

- Matthias's Rules for Superconductors
  … "Stay away from Theorists"
  Team up with theorists
  (and provide them with useful feedback
  e.g., Thin-Film Synthesis + ARPES)

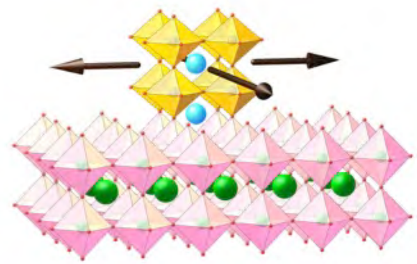
Why Thin-Film Synthesis + ARPES ?

"Artificial" Quantum Materials

Interface Engineering

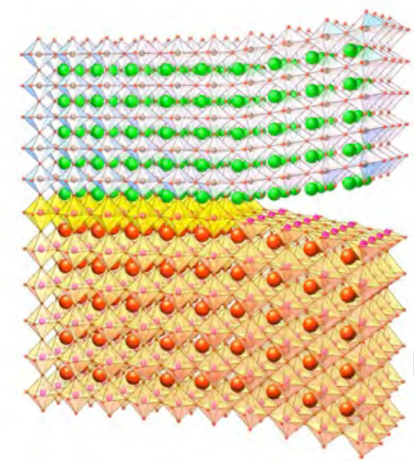


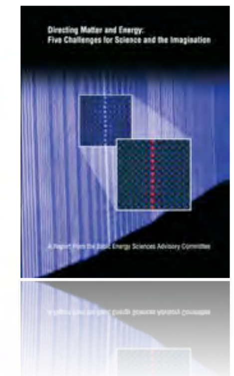
$(LaMnO_3)_{2n}$ / $(SrMnO_3)_n$



Strain Engineering

FeSe / $SrTiO_3$



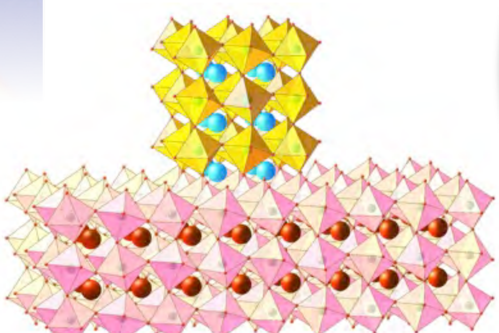


$LaAlO_3$ / $SrTiO_3$
Bi_2Se_3 / EuS

Polarization Doping & Proximity Effects (from juxtaposed competing ground states)

Bulk Quantum Materials

ARPES



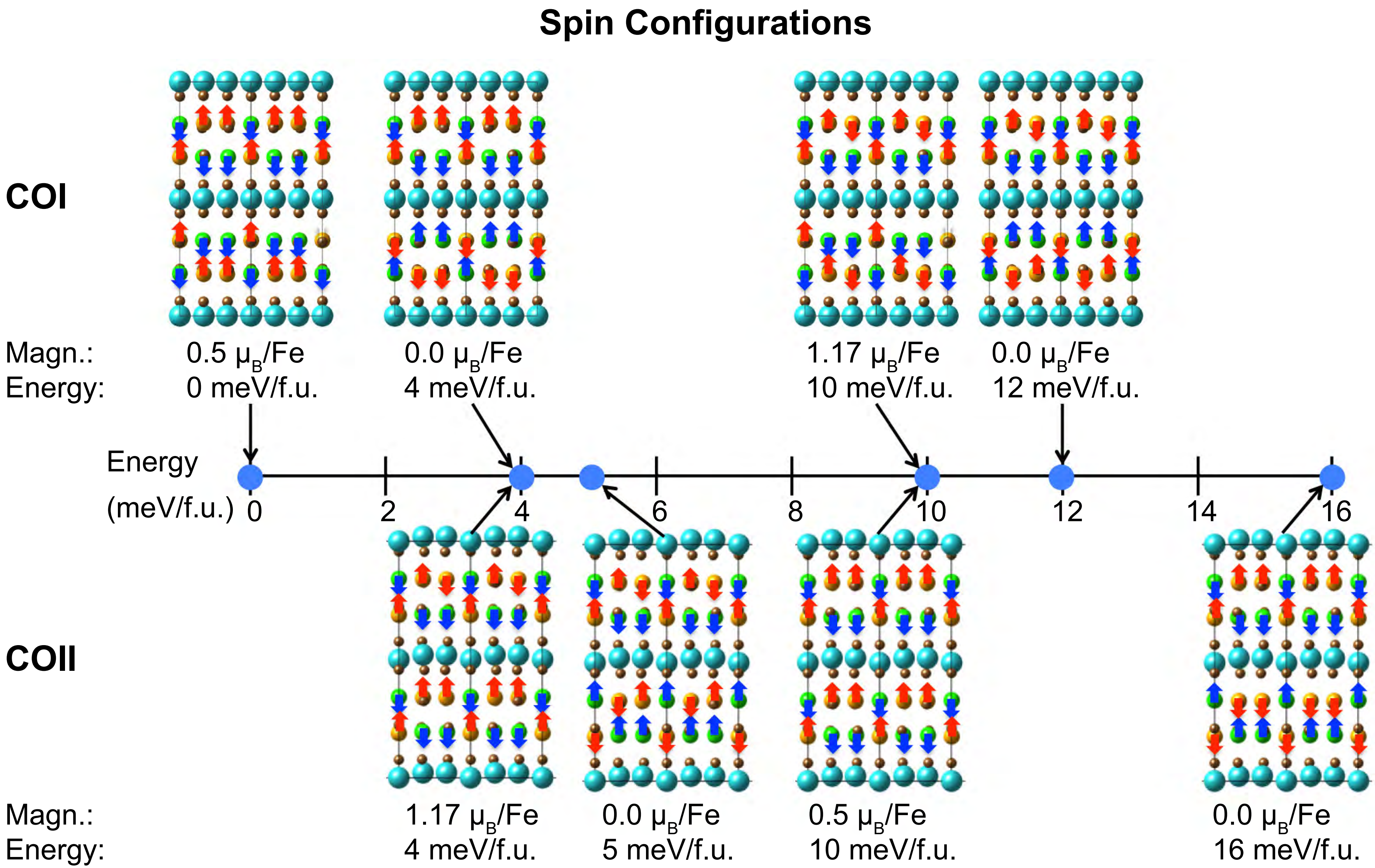
Epitaxial Stabilization

$BaRuO_3$ / $SrTiO_3$
Ba_2RuO_4 / $GdScO_3$

Dimensional Confinement

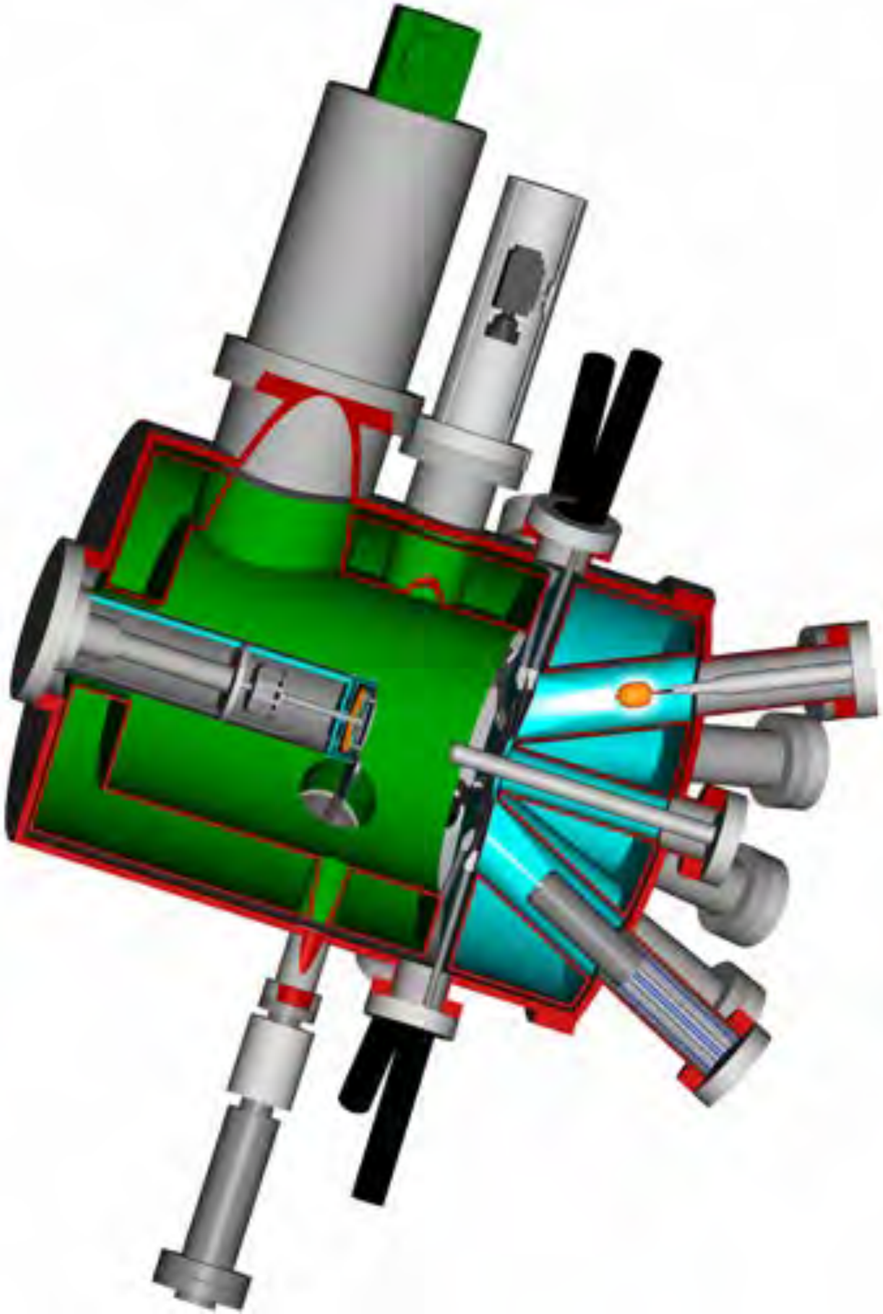
$A_{n+1}B_nO_{3n+1}$: $(La,Sr)_2CuO_4$, Sr_2RuO_4, Sr_2IrO_4

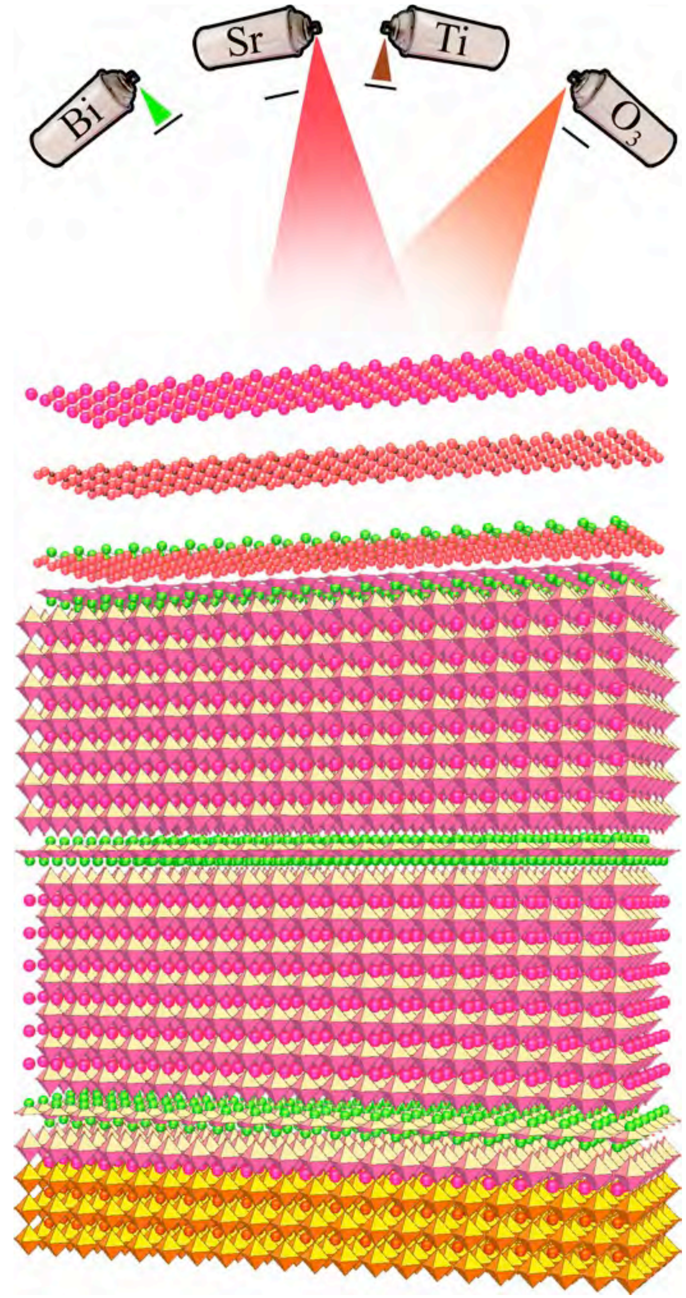
Example—Hidden Phases of $LuFe_2O_4$



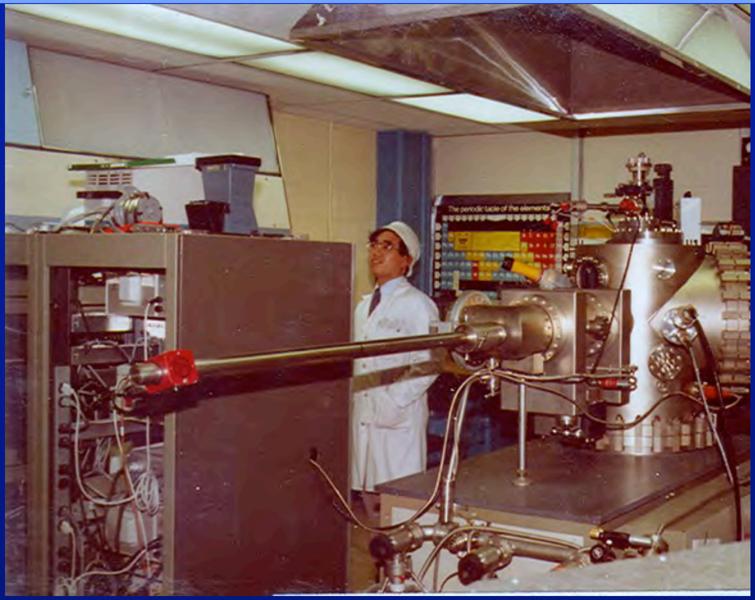
J.A. Mundy, C.M. Brooks, M.E. Holtz, J.A. Moyer, H. Das, A.F. Rébola, J.T. Heron, J.D. Clarkson, S.M. Disseler, Z. Liu, A. Farhan, R. Held, R. Hovden, E. Padgett, Q. Mao, H. Paik, R. Misra, L.F. Kourkoutis, E. Arenholz, A. Scholl, J.A. Borchers, W.D. Ratcliff, R. Ramesh, C.J. Fennie, P. Schiffer, D.A. Muller, and D.G. Schlom, *Nature* **537** (2016) 523–527.

MBE ≈ Atomic Spray Painting

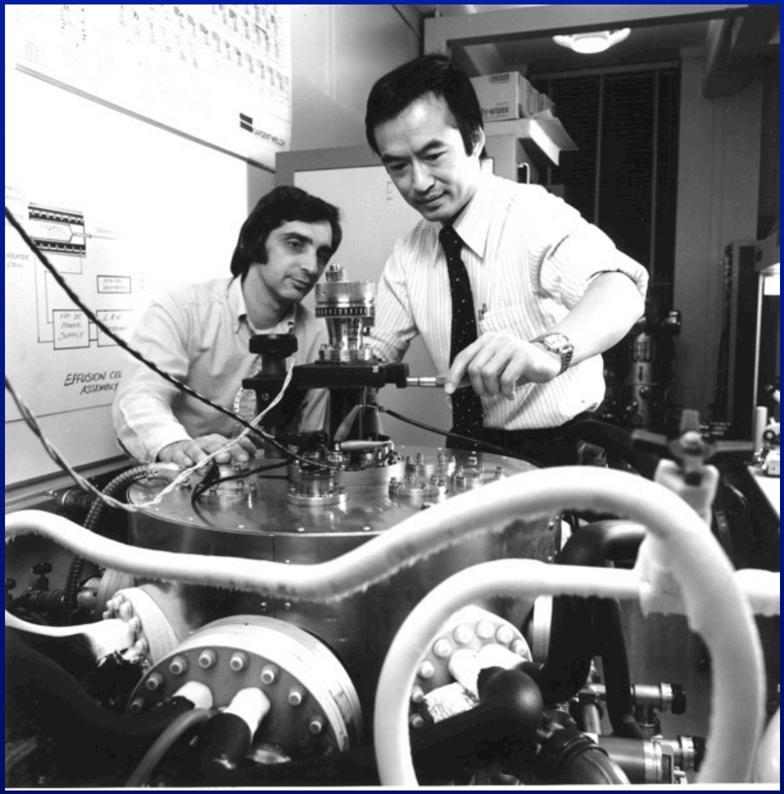




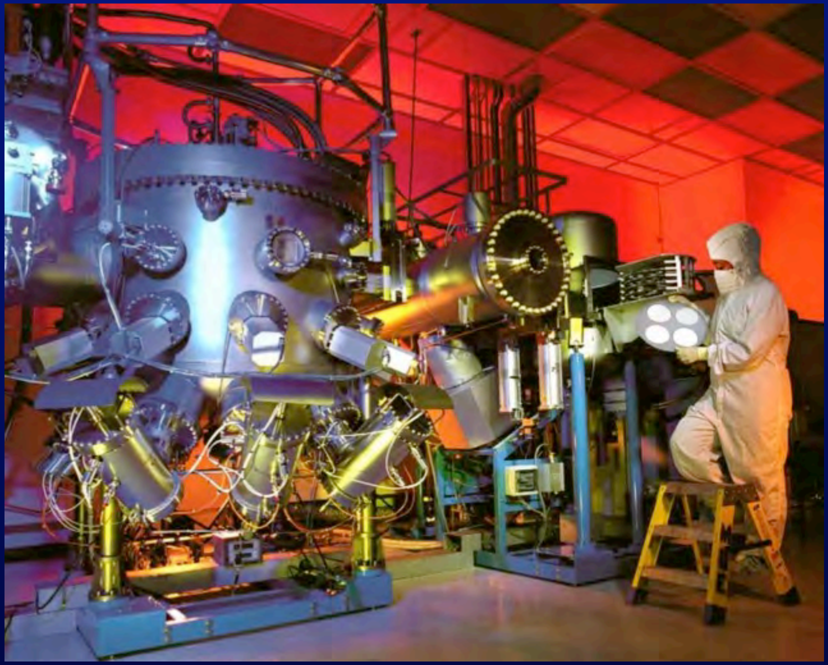
Evolution of MBE



1st University MBE Cornell, 1978

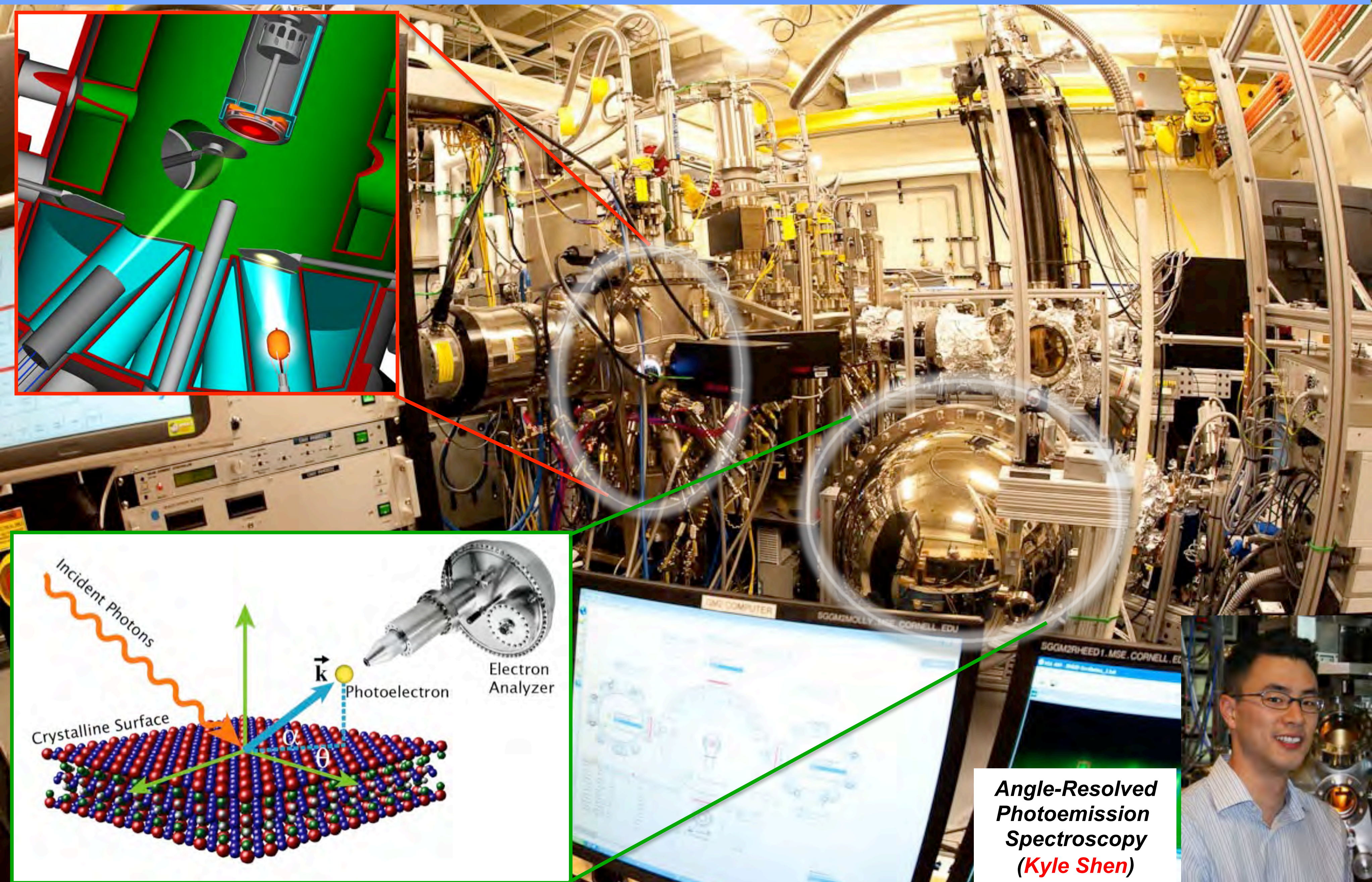


1st MBE
Al Cho at Bell Labs, 1972



Production MBE Today
(courtesy of TRW)

Oxide MBE + ARPES



MBE + ARPES

Titanates

$SrTiO_3$
Sr_2TiO_4
$LaTiO_3$

Vanadates

$SrVO_3$
$LaVO_3$
$SrVO_3$ / $LaVO_3$

Manganites

$La_{1-x}Sr_xMnO_3$
$SrMnO_3$
$LaMnO_3$ / $SrMnO_3$

Nickelates

$LaNiO_3$

Cuprates

La_2CuO_4 *T'*
$Sr_{1-x}La_xCuO_2$

Ruthenates

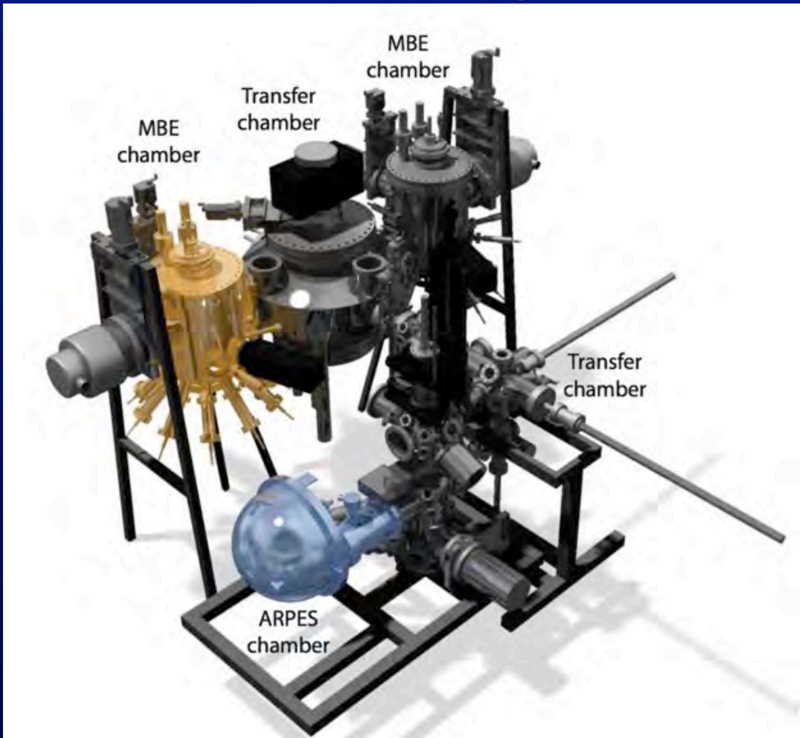
RuO_2
$SrRuO_3$
Sr_2RuO_4
$BaRuO_3$
Ba_2RuO_4
$CaRuO_3$
Ca_2RuO_4
$Pb_2Ru_2O_{6.5}$

Iridates

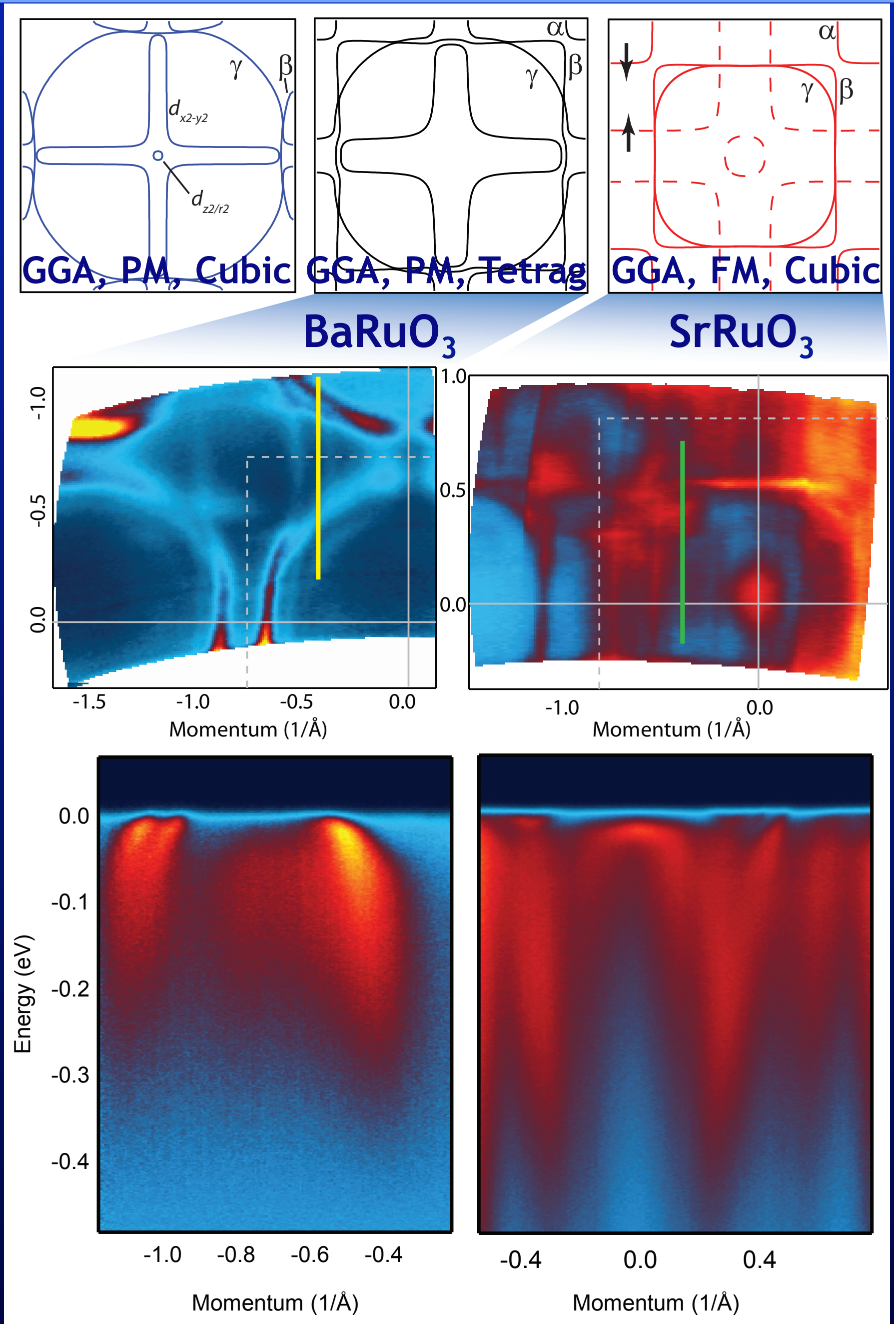
IrO_2
IrO_2 / TiO_2
$SrIrO_3$
Sr_2IrO_4
Ba_2IrO_4
$Bi_2Ir_2O_7$

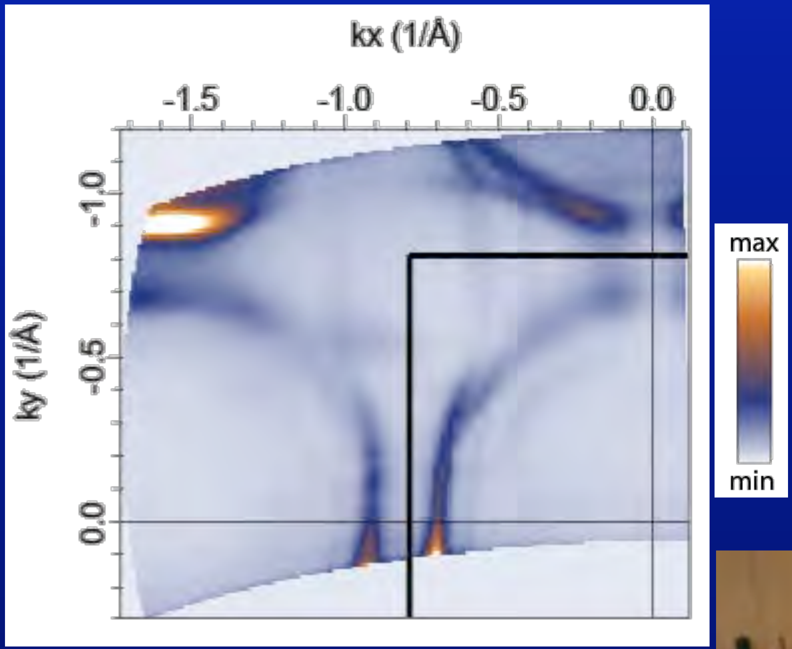
Other Materials

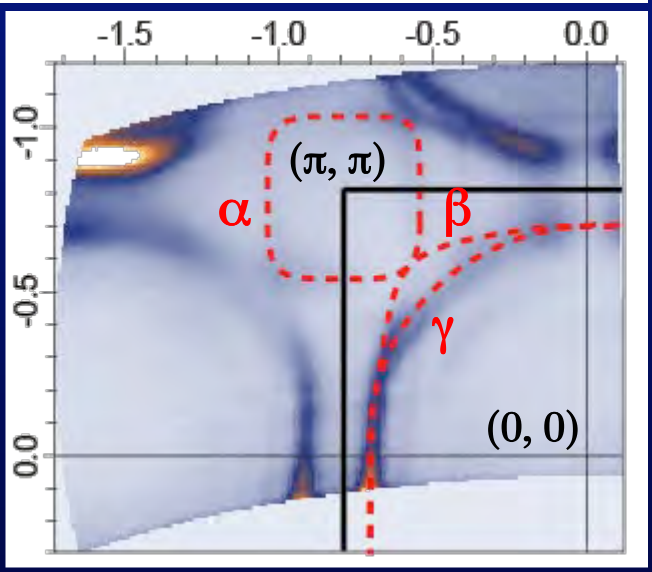
$YbAl_3$
$LuAl_3$
$YbAl_3$ / $LuAl_3$
$BaBiO_3$
$BaSnO_3$
$BaPbO_3$
FeSe

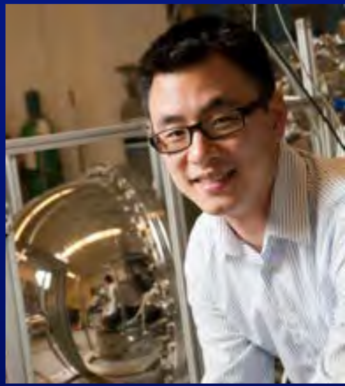


ARPES of $BaRuO_3$ / $SrTiO_3$





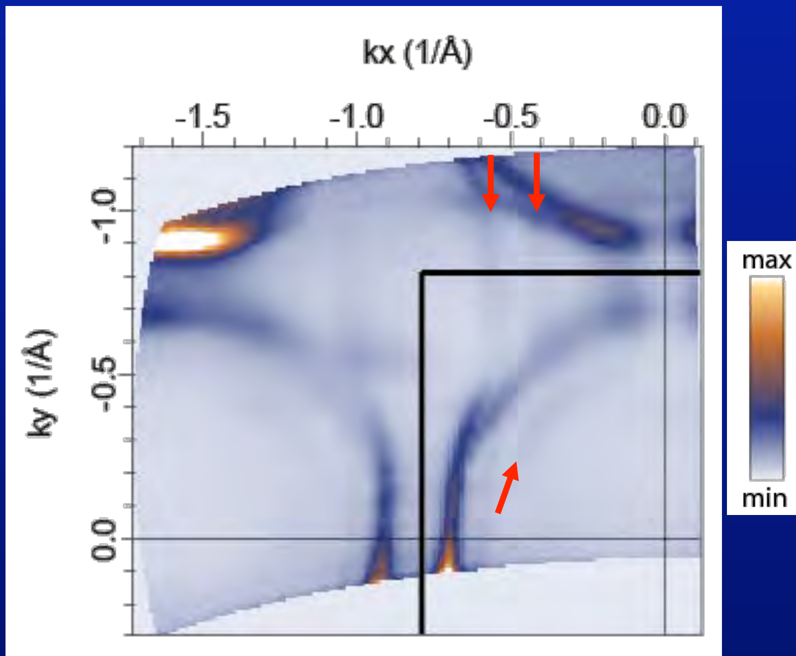


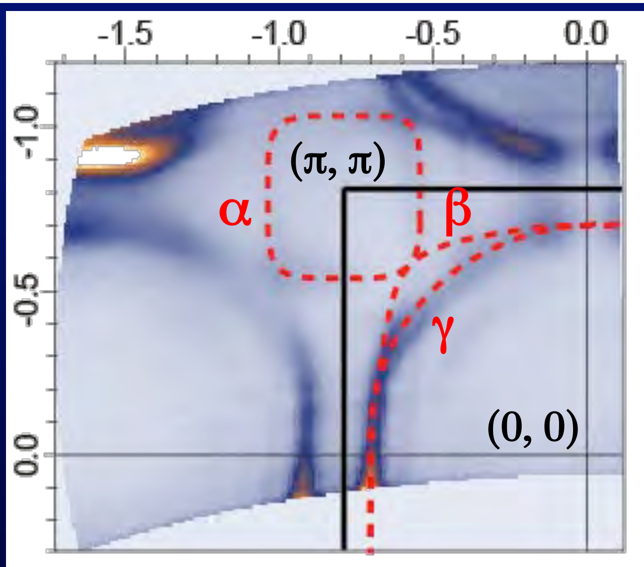


Kyle Shen

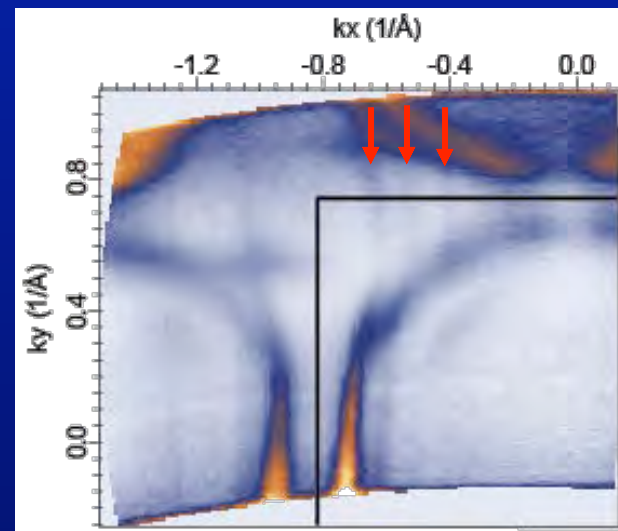
Quantum Well States in $BaRuO_3$

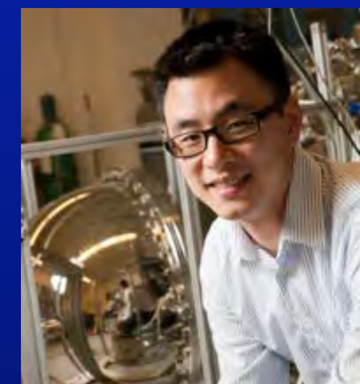
Thickness 3 unit cells





Thickness 4 unit cells

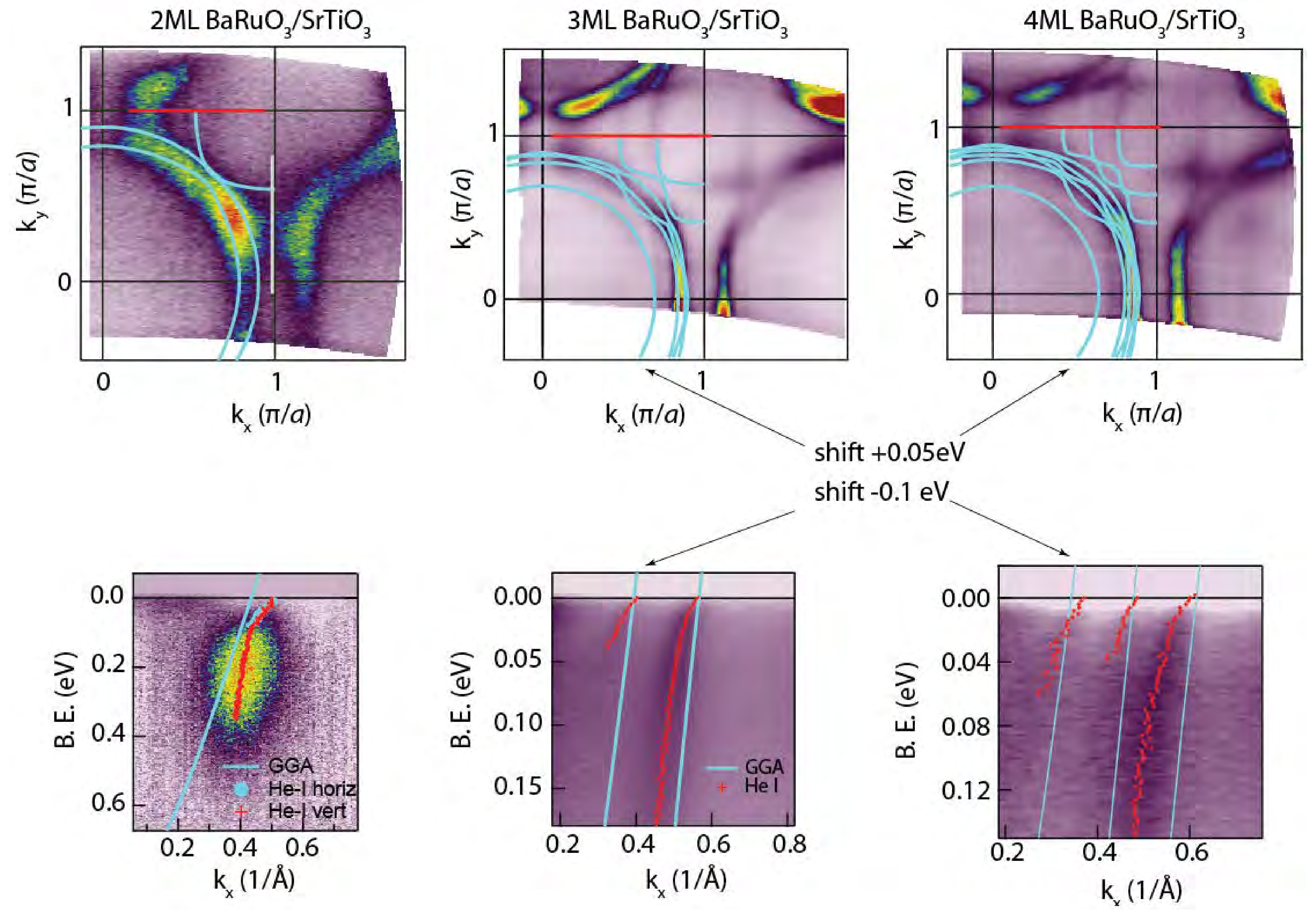




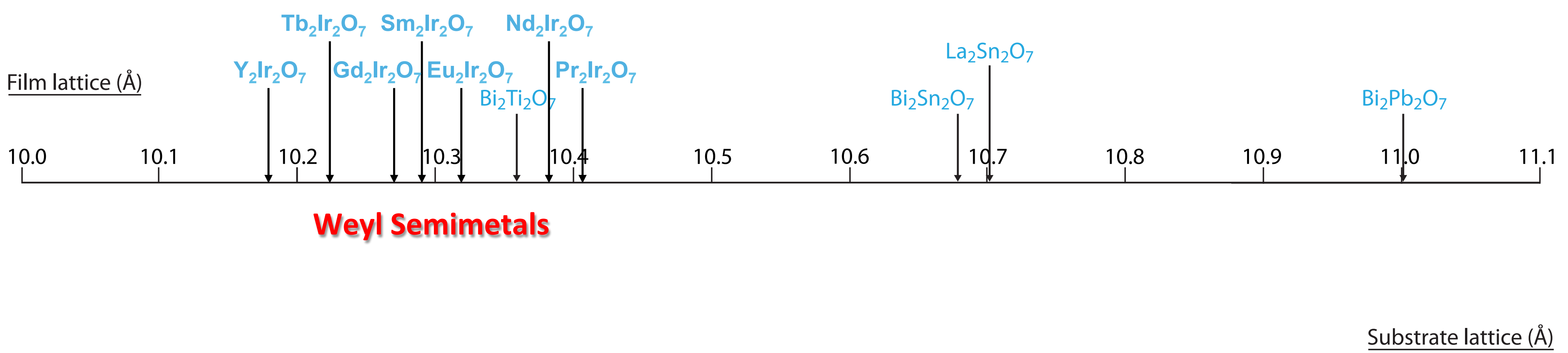
Kyle Shen

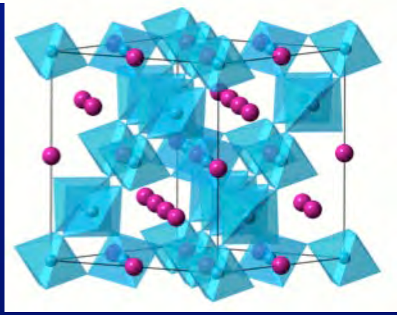
- FM suppressed because of finite thickness?
- Or tetragonal distortion?

Thickness Dependence

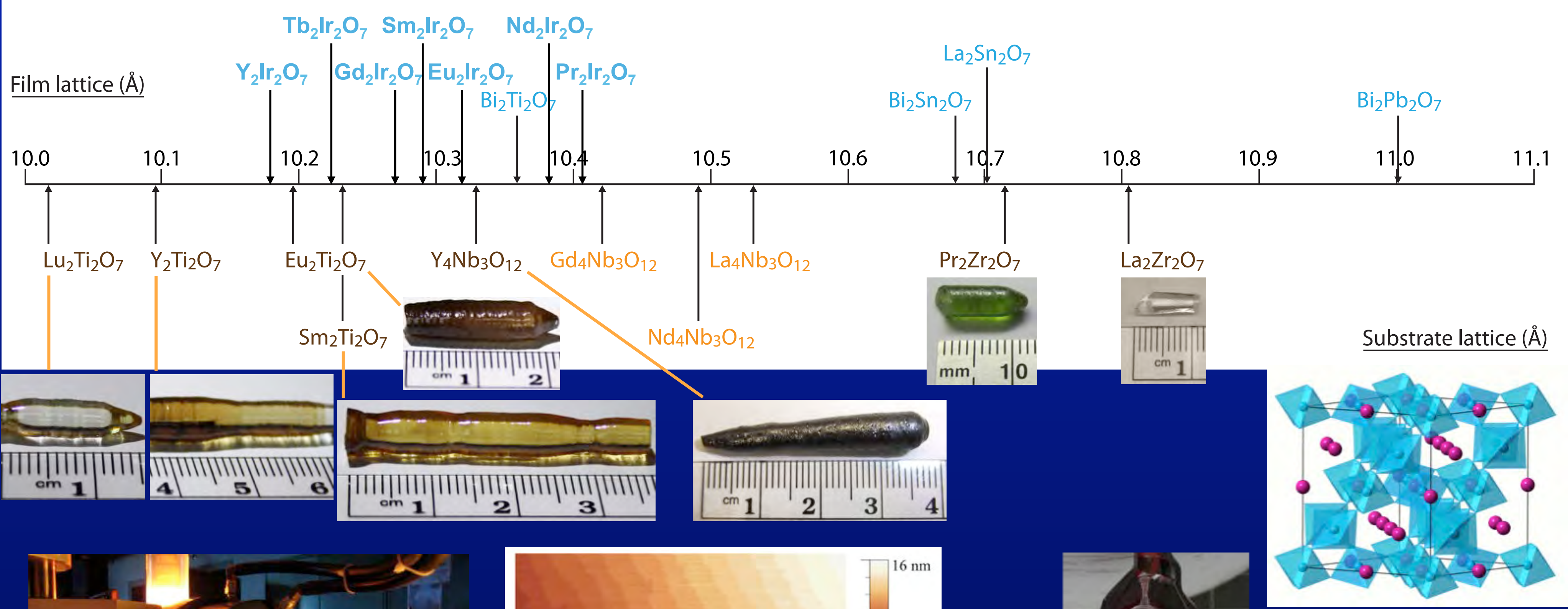


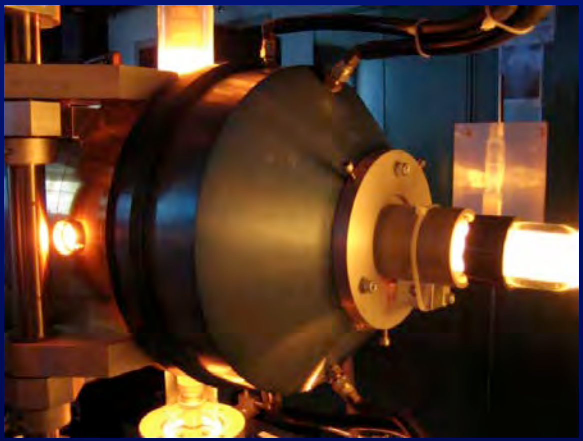
How about Pyrochlores?



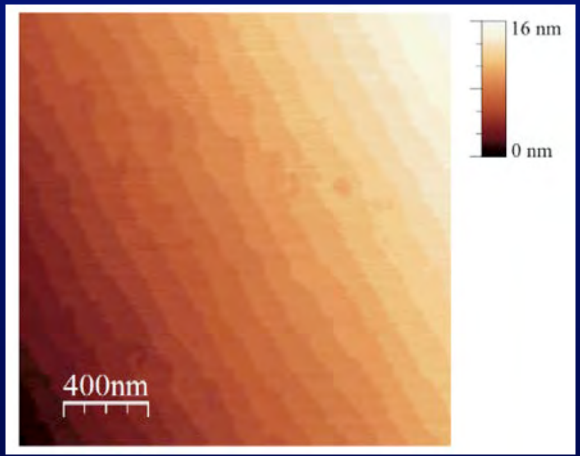


Pyrochlore Substrates





Floating zone furnace (Augsburg)



AFM: as-polished (111) $Sm_2Ti_2O_7$ (floating zone)

$Sm_2Ti_2O_7$ grown by Czochralski (IKZ, Berlin)

Tyrel McQueen

BREAK THE RULES

- Gibbs' Rule
  $\Delta G < 0$ to form stable phases
  Exploit interfacial energy from substrate

- Matthias's Rules for Superconductors
  … "Stay away from Theorists"
  Team up with theorists
  (and provide them with useful feedback)

- Pauling's Rules for Crystal Structures
  Radius ratio criteria for stability

Pauling's Rules

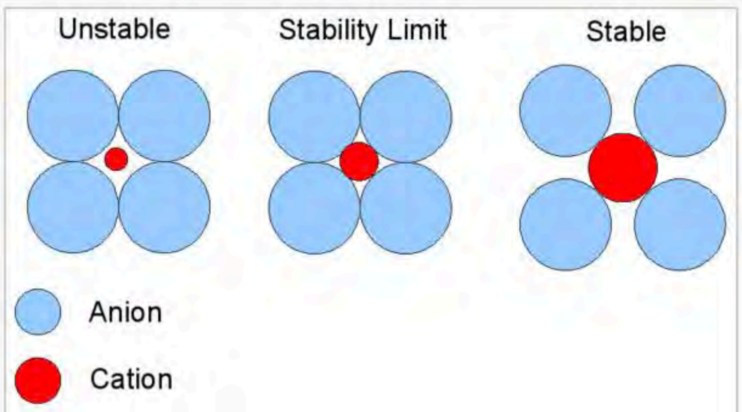
First rule: the radius ratio rule [edit]

For typical ionic solids, the cations are smaller than the anions, and each cation is surrounded by coordinated anions which form a polyhedron. The sum of the ionic radii determines the cation-anion distance, while the cation-anion radius ratio r_+/r_- (or r_c/r_a) determines the coordination number (C.N.) of the cation, as well as the shape of the coordinated polyhedron of anions.[3][4]

For the coordination numbers and corresponding polyhedra in the table below, Pauling mathematically derived the *minimum* radius ratio for which the cation is in contact with the given number of anions (considering the ions as rigid spheres). If the cation is smaller, it will not be in contact with the anions which results in instability leading to a lower coordination number.

Polyhedron and minimum radius ratio for each coordination number

C.N.	Polyhedron	Radius ratio
3	triangular	0.155
4	tetrahedron	0.225
6	octahedron	0.414
7	capped octahedron	0.592
8	square antiprism (anticube)	0.645
8	cube	0.732
9	triaugmented triangular prism	0.732
12	cuboctahedron	1.00



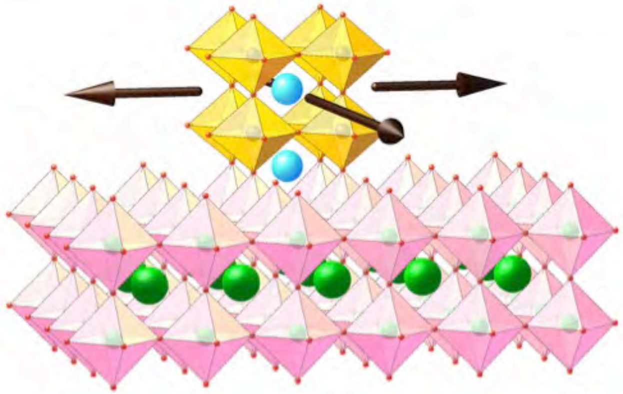
Critical Radius Ratio. This diagram is for coordination number six: 4 anions in the plane shown, 1 above the plane and 1 below. The stability limit is at $r_C/r_A = 0.414$

https://en.wikipedia.org/wiki/Pauling%27s_rules

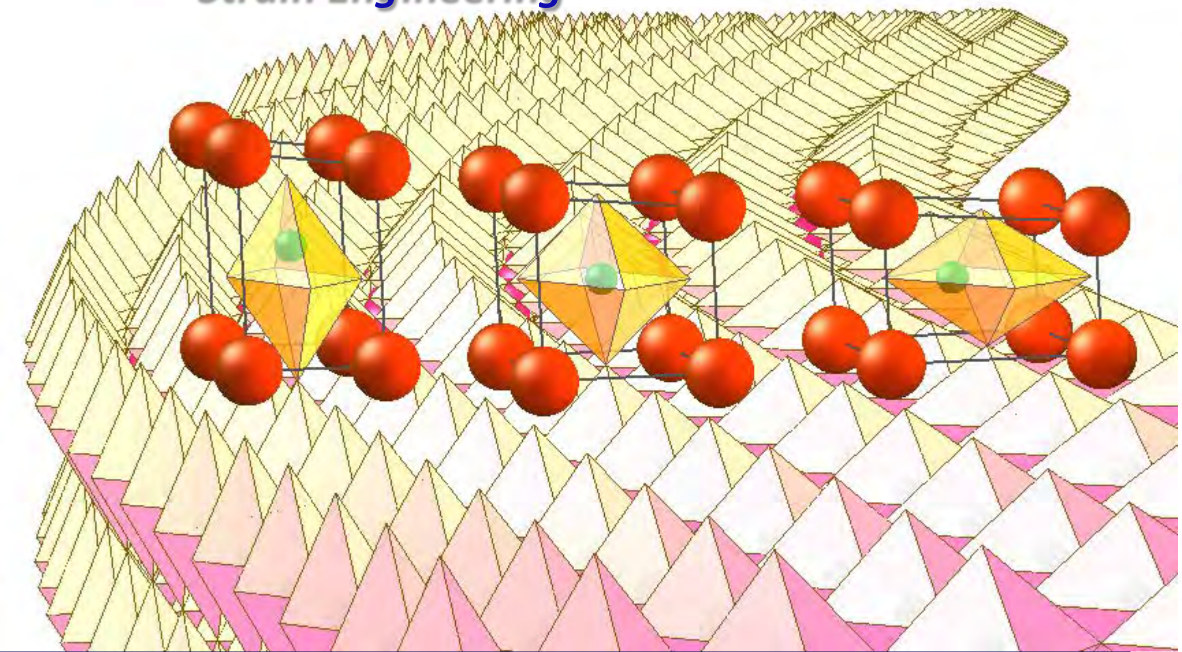
A. Magnus, "Über chemische Komplexverbindungen," *Z. Anorg. Allg. Chem.* **124** (1922) 289–321.

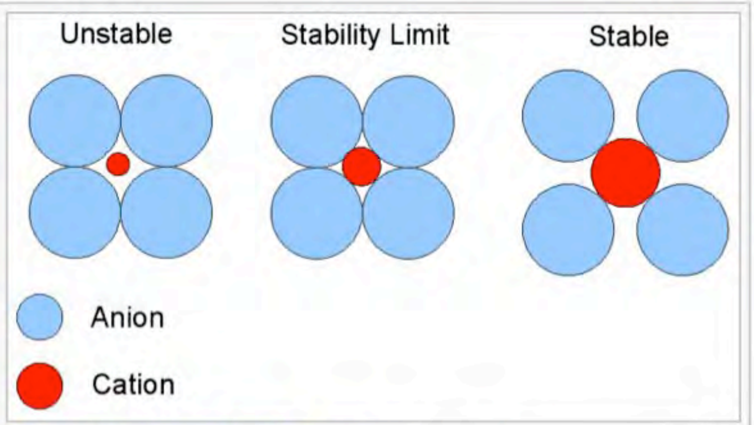
L. Pauling, "The Principles Determining the Structure of Complex Ionic Crystals," *J. Am. Chem. Soc.* **51** (1929) 1010–1026.

BREAK Pauling's Rules



Strain Engineering





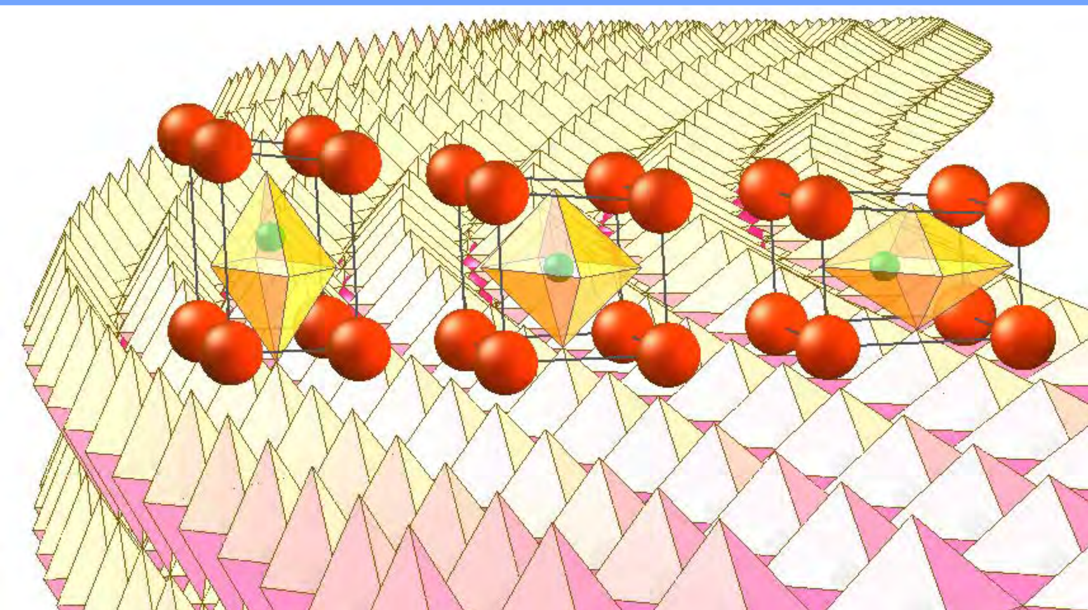
Critical Radius Ratio. This diagram is for coordination number six: 4 anions in the plane shown, 1 above the plane and 1 below. The stability limit is at $r_C/r_A = 0.414$

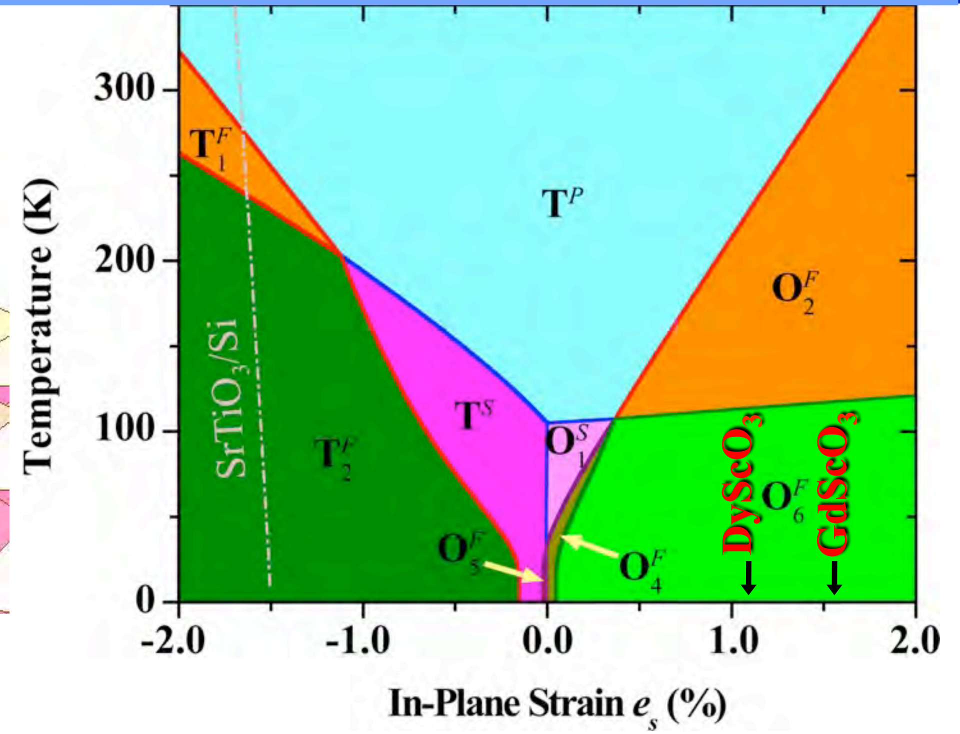
https://en.wikipedia.org/wiki/Pauling%27s_rules

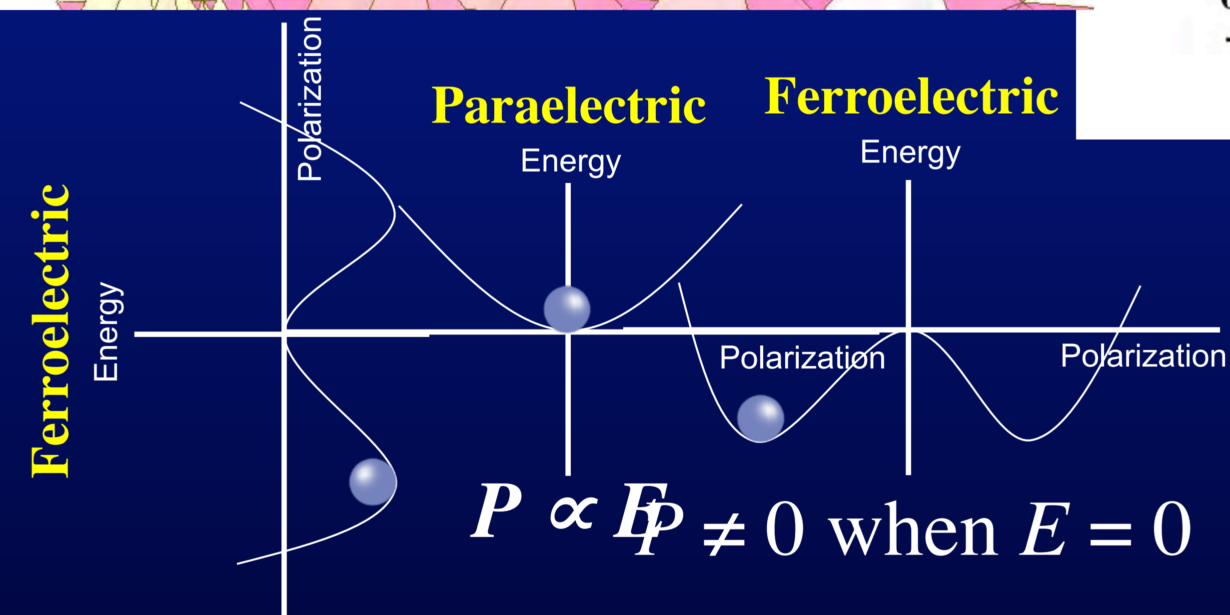
A. Magnus, "Über chemische Komplexverbindungen," *Z. Anorg. Allg. Chem.* **124** (1922) 289–321.

L. Pauling, "The Principles Determining the Structure of Complex Ionic Crystals," *J. Am. Chem. Soc.* **51** (1929) 1010–1026.

Strained $SrTiO_3$—Transmuting a Dielectric into a Ferroelectric

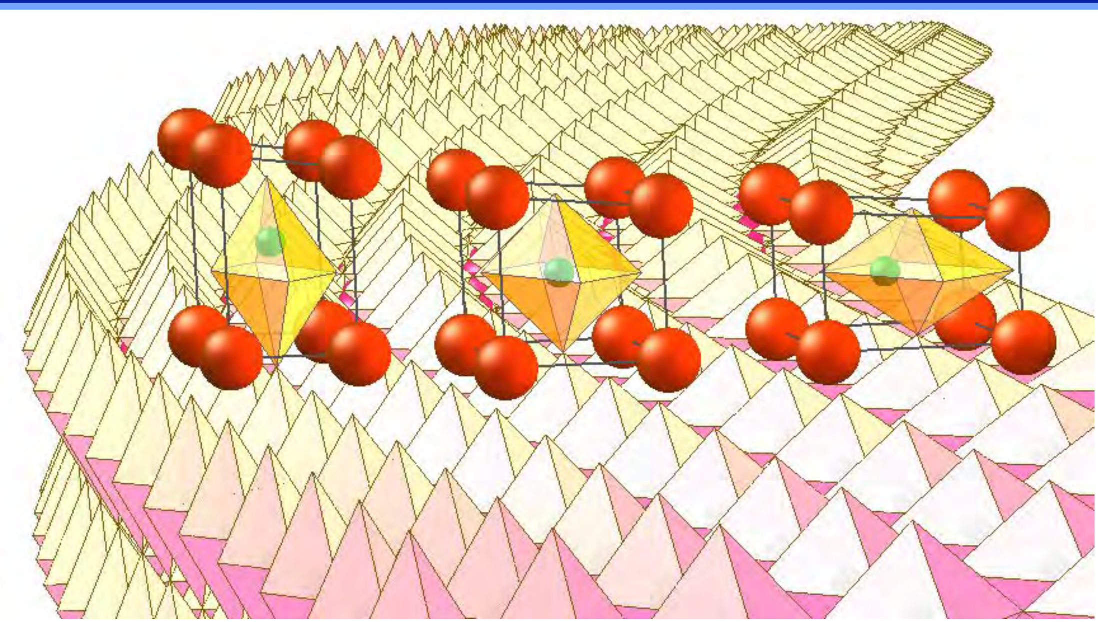


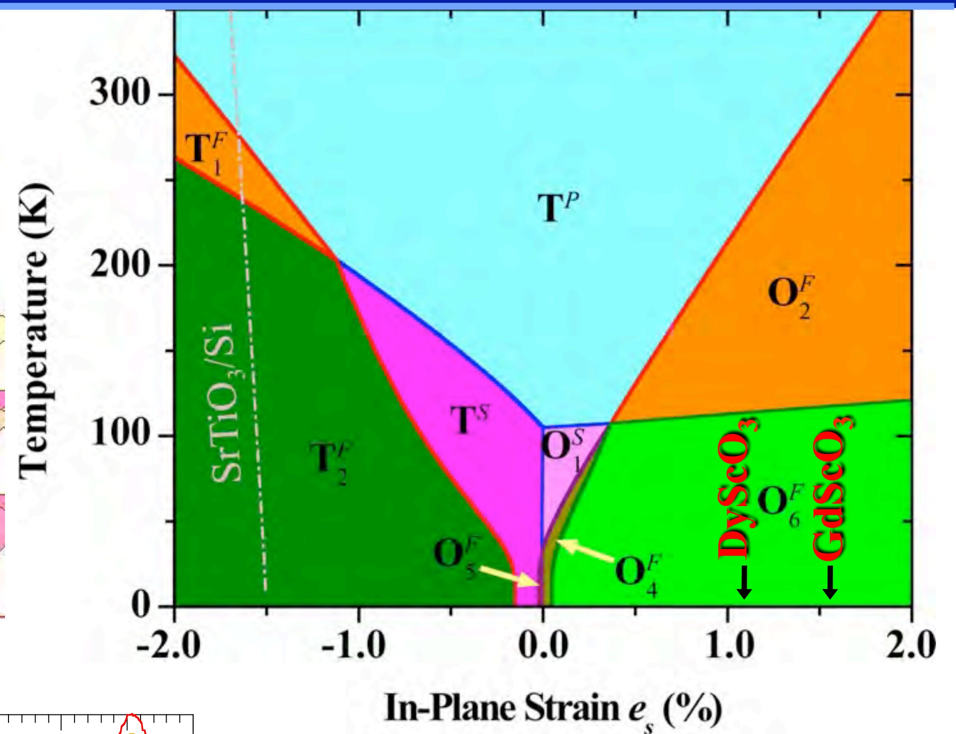


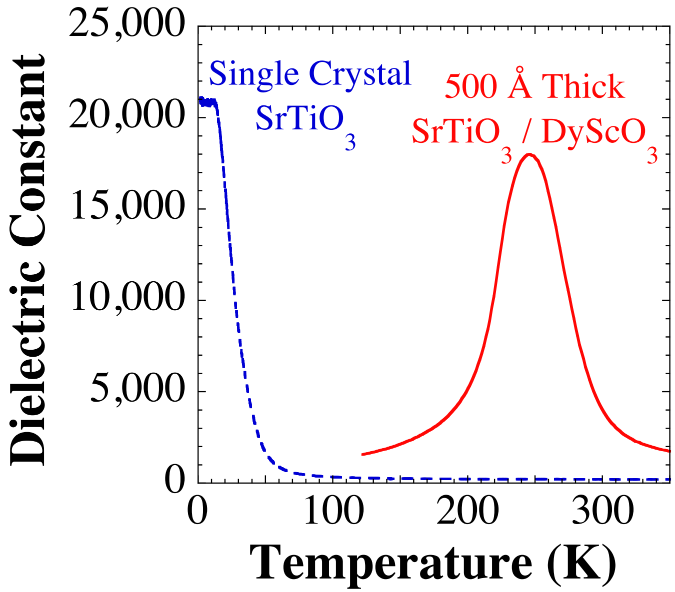


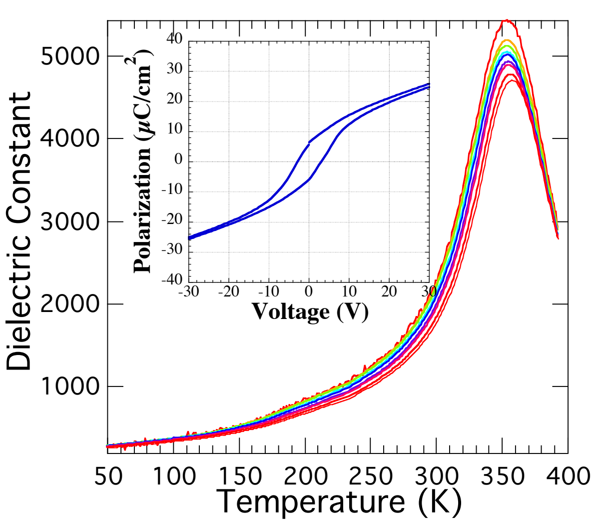
N.A. Pertsev, A.K. Tagantsev, and N. Setter, *Physical Review* **61** (2000) 825-829.

Strained $SrTiO_3$—Transmuting a Dielectric into a Ferroelectric







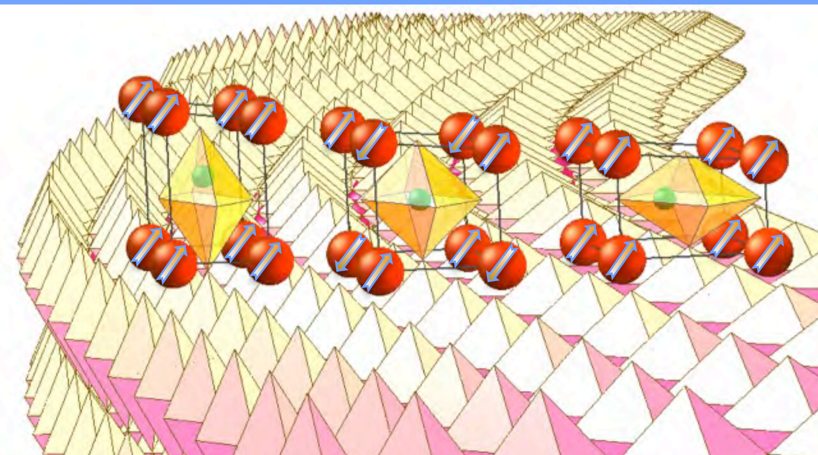


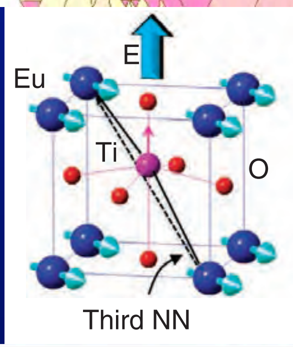
N.A. Pertsev, A.K. Tagantsev, and N. Setter, *Physical Review* **61** (2000) 825-829.

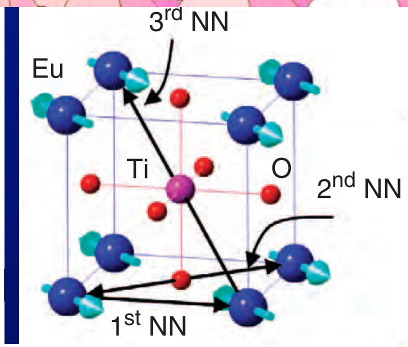
Ferroelectric at Room Temperature

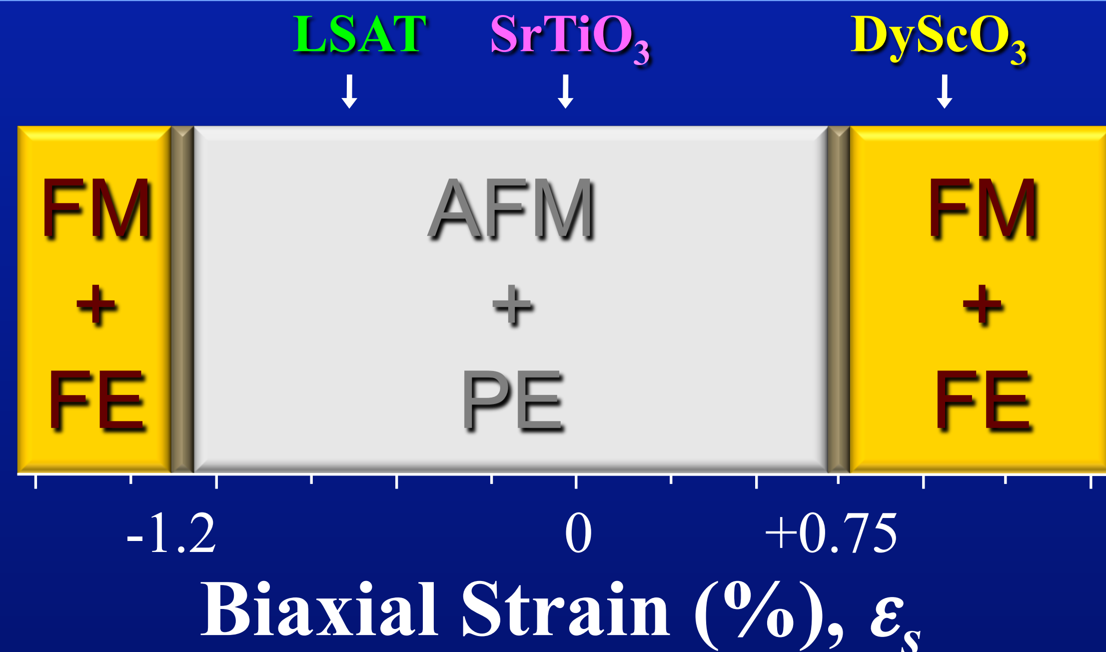
J.H. Haeni, P. Irvin, W. Chang, R. Uecker, P. Reiche, Y.L. Li, S. Choudhury, W. Tian, M.E. Hawley, B. Craigo, A.K. Tagantsev, X.Q. Pan, S.K. Streiffer, L.Q. Chen, S.W. Kirchoefer, J. Levy, and D.G. Schlom, *Nature* **430** (2004) 758–761.

Strained $EuTiO_3$—Strongest Ferromagnetic Ferroelectric









C.J. Fennie and K.M. Rabe
Physical Review Letters **97** (2006)

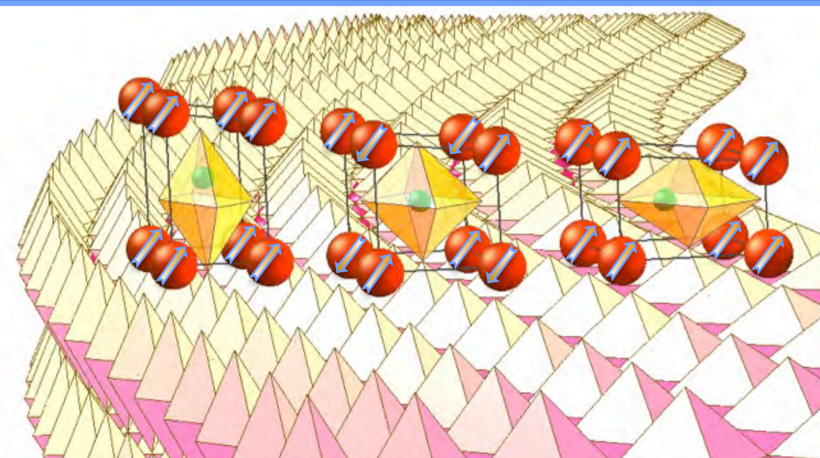
P.J. Ryan, J.-W. Kim, T. Birol, P. Thompson, J.-H. Lee, X. Ke, P.S. Normile, E. Karapetrova, P. Schiffer, S.D. Brown, C.J. Fennie, and D.G. Schlom
Nature Communications 4 (2013) 1334.

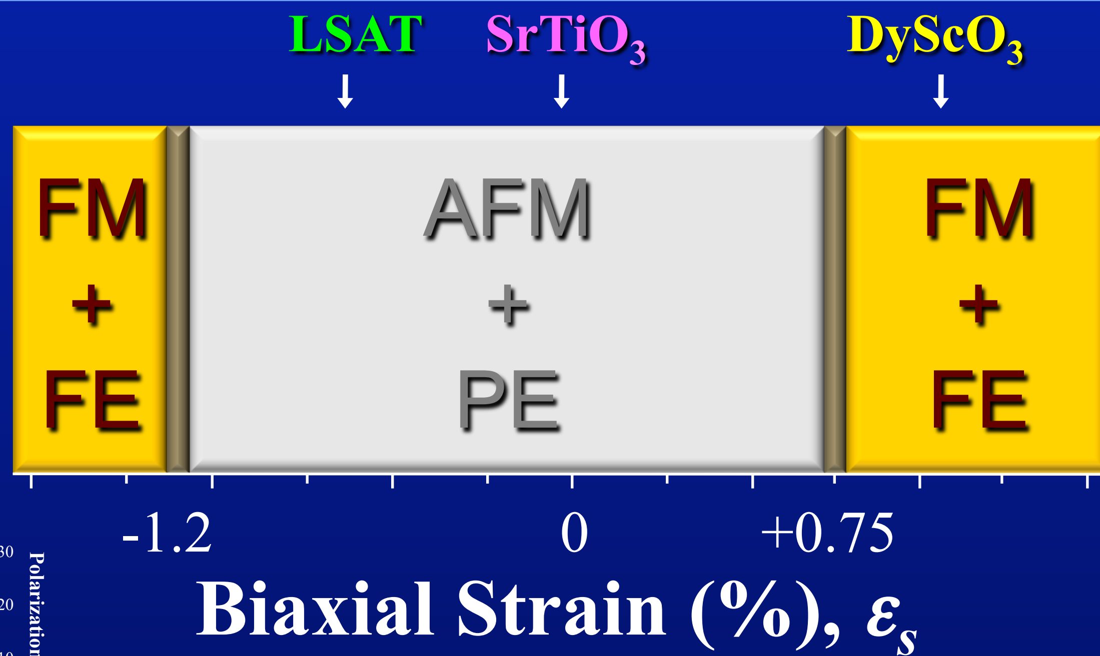
Table 1 | Calculated magnetic exchange constants.

ETO–LSAT	J_{1xy}	J_{1z}	J_{2xy}	J_{2z}	J_3
J/K_B(K)–bulk	+0.075	−0.114	+0.062	+0.083	−0.031
# Neighbours	4	2	4	8	8
J/K_B(K)–LSAT	+0.086	−0.147	+0.06	+0.087	−0.034

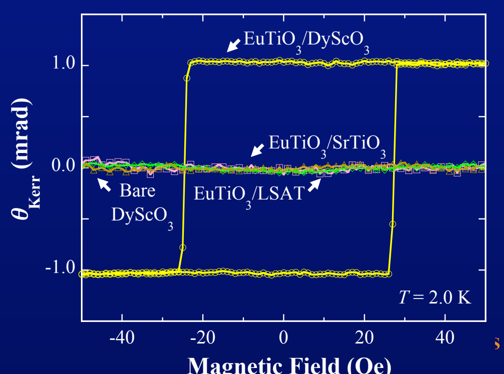
Shown are the exchange constants (J) calculated between the Eu ions within the unconstrained bulk I4/mcm ETO and the ETO film on LSAT with ($a^0a^0c^-$) structure under −0.9% compressive strain, including the first, second and third NN Eu ions describing both the in-plane (xy) and out-of-plane (z) interactions. Positive indicates FM and negative AFM coupling. The second row indicates the number of neighbours for each particular interaction. The first and second NN interactions are mostly FM bar the first NN out-of-plane J_{1z} exchange constant. The calculations indicate the importance of J_3 in determining the G-AFM structure in ETO.

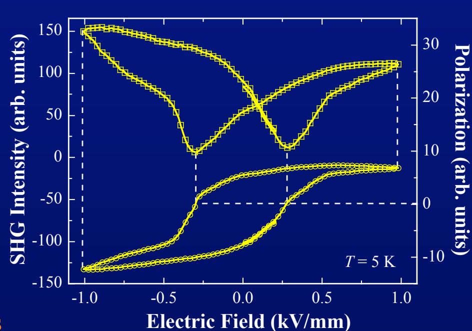
Strained EuTiO$_3$—Strongest Ferromagnetic Ferroelectric





C.J. Fennie and K.M. Rabe *Physical Review Letters* **97** (2006) 267602.

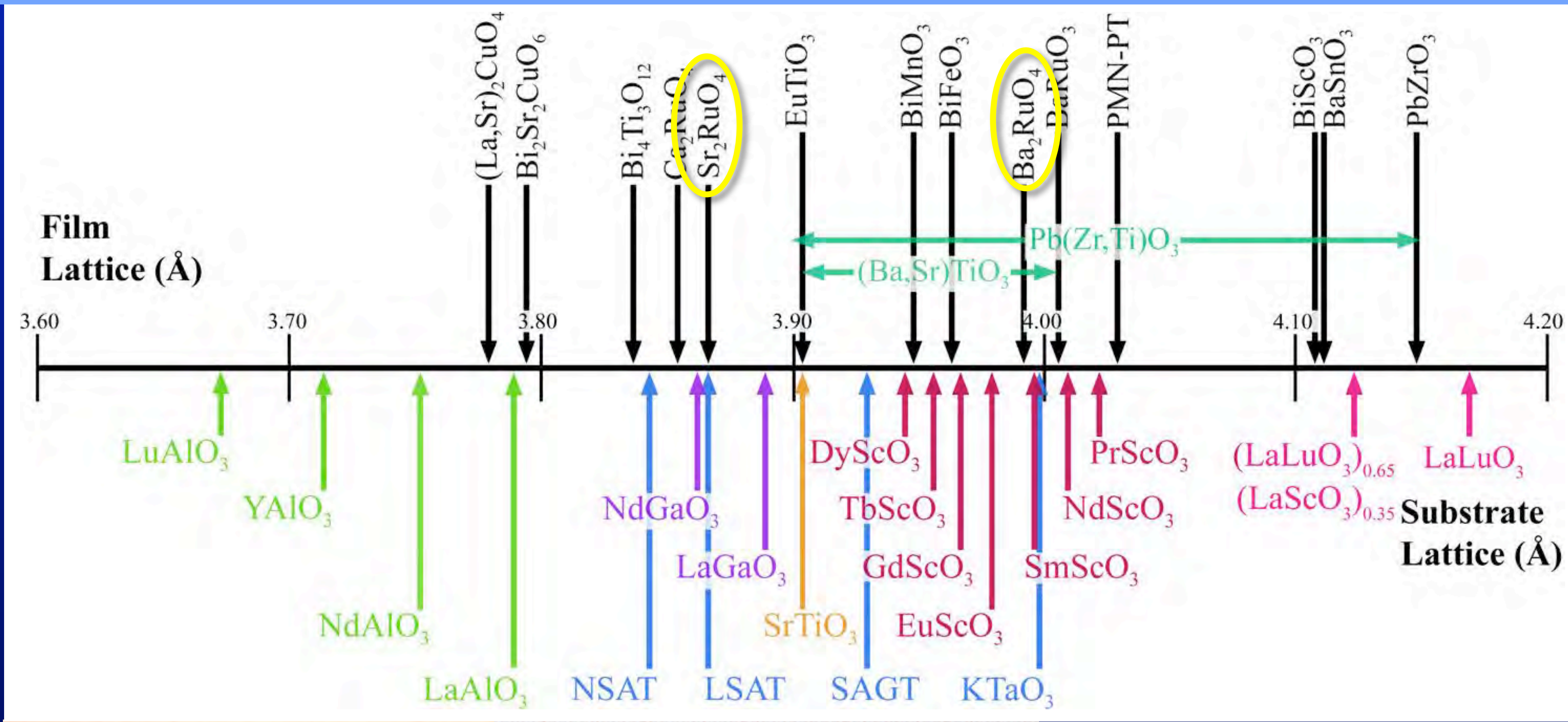


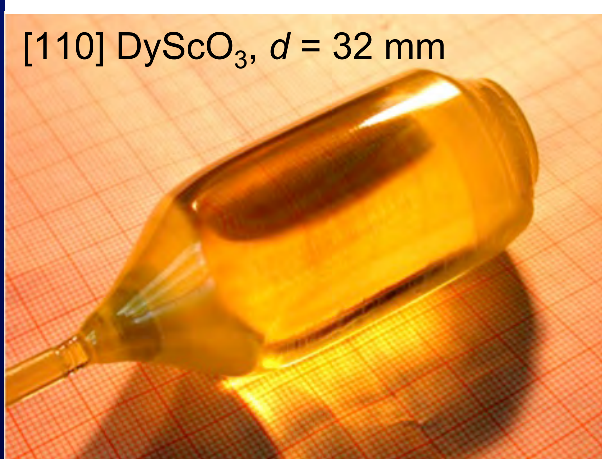


22 nm thick EuTiO$_3$ (a boring dielectric) **+ 1.1% Strain** (by growing it commensurately) **= Multiferroic** (1000× stronger than prior ferromagnetic ferroelectrics)

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.

Commercial Perovskite Substrates

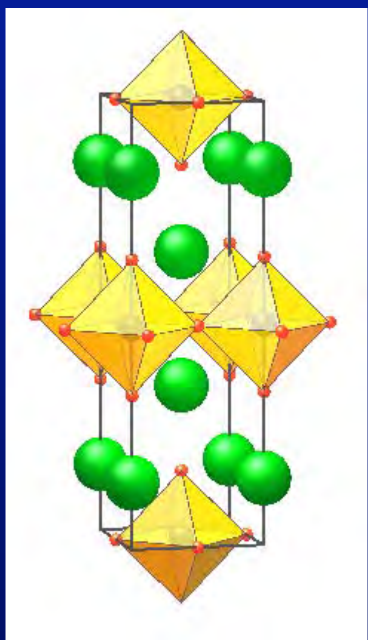




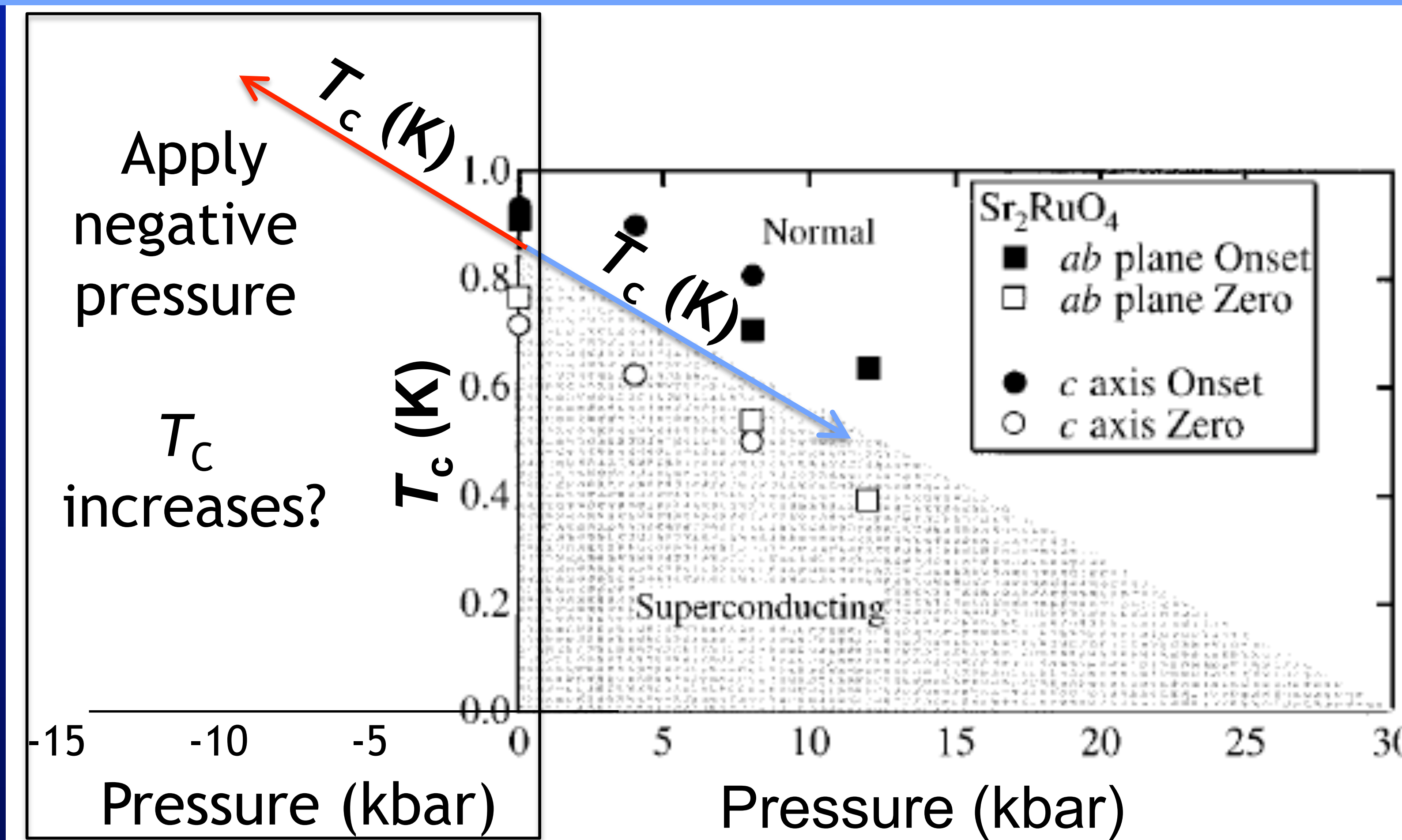
D.G. Schlom, L.Q. Chen, C.J. Fennie, V. Gopalan, D.A. Muller, X.Q. Pan, R. Ramesh, and R. Uecker, "Elastic Strain Engineering of Ferroic Oxides," *MRS Bulletin* **39** (2014) 118-130.

Effect of Strain on Sr_2RuO_4 (a spin-triplet superconductor)

Sr_2RuO_4



n = 1

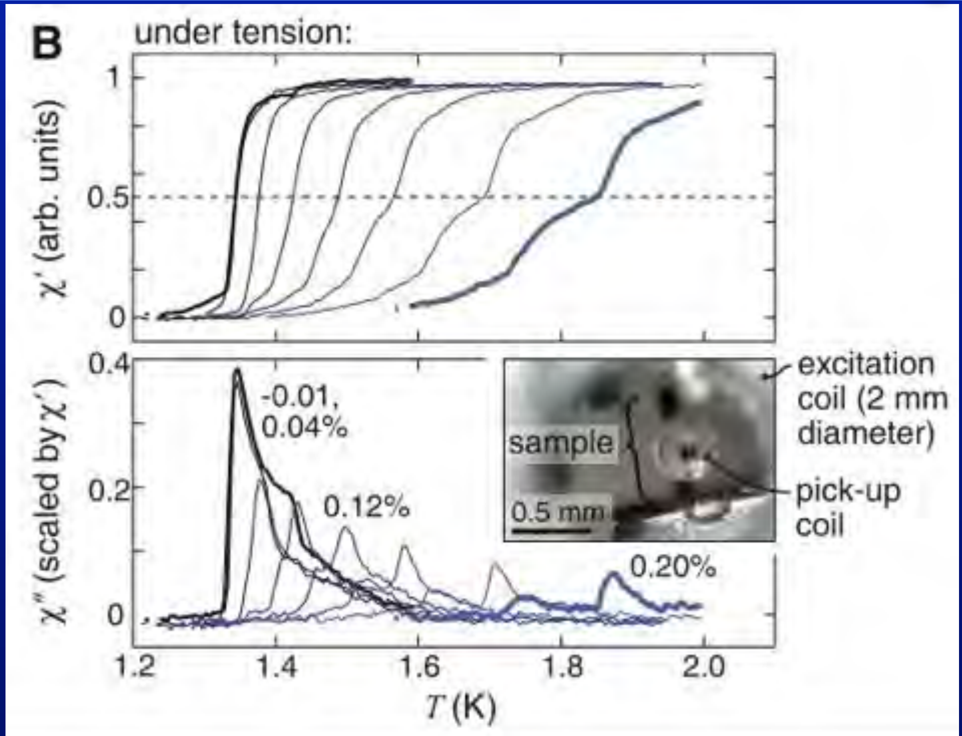


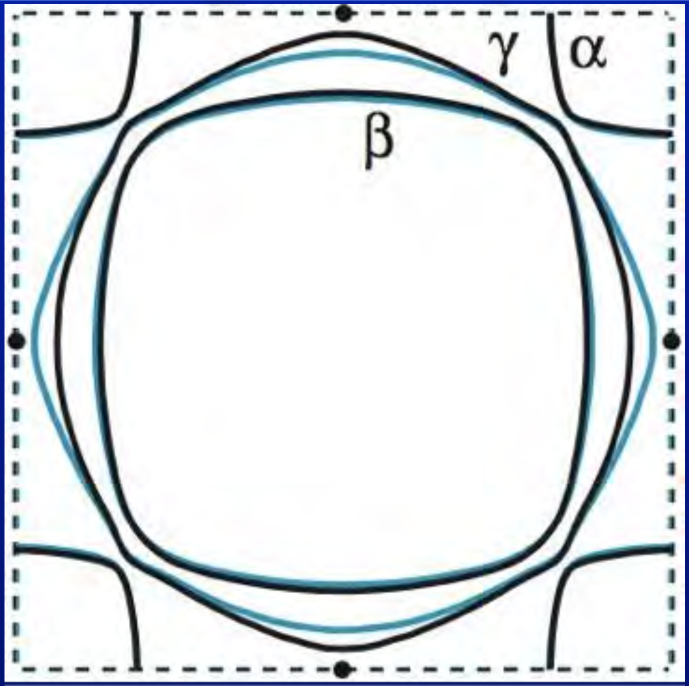
T_C goes down with increasing pressure

→ apply negative pressure

N. Shirakawa, K. Murata, S. Nishizaki, Y. Maeno, T. Fujita, *Phys. Rev. B* **56** (1997) 7890-7893.

In-plane Uniaxial Strain Dramatically Increases T_c in Sr_2RuO_4



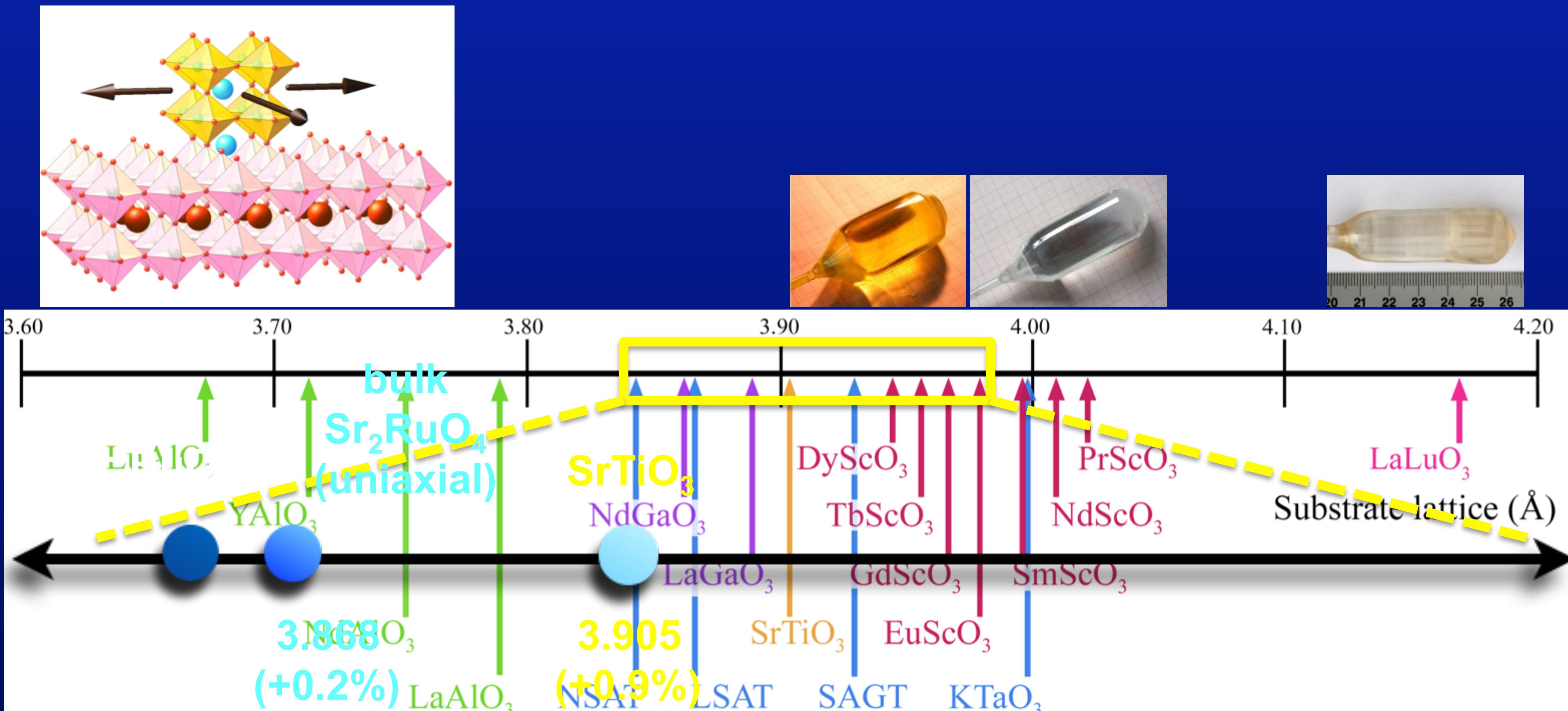


0.5% strain along [100]

enhancements in T_c may be tied to proximity of van Hove singularity to E_F, but strains that can be applied to single crystal Sr_2RuO_4 are relatively modest (≤ 0.8%; $T_{c,max}$ of 3.4 K at 0.6% uniaxial compressive strain)

C.W. Hicks, D.O. Brodsky, E.A. Yelland, A.S. Gibbs, J.A.N. Bruin, M.E. Barber, S.D. Edkins, K. Nishimura, S. Yonezawa, Y. Maeno, and A.P. Mackenzie, *Science* **344** (2014) 283–285.
+ arXiv:1604.06669

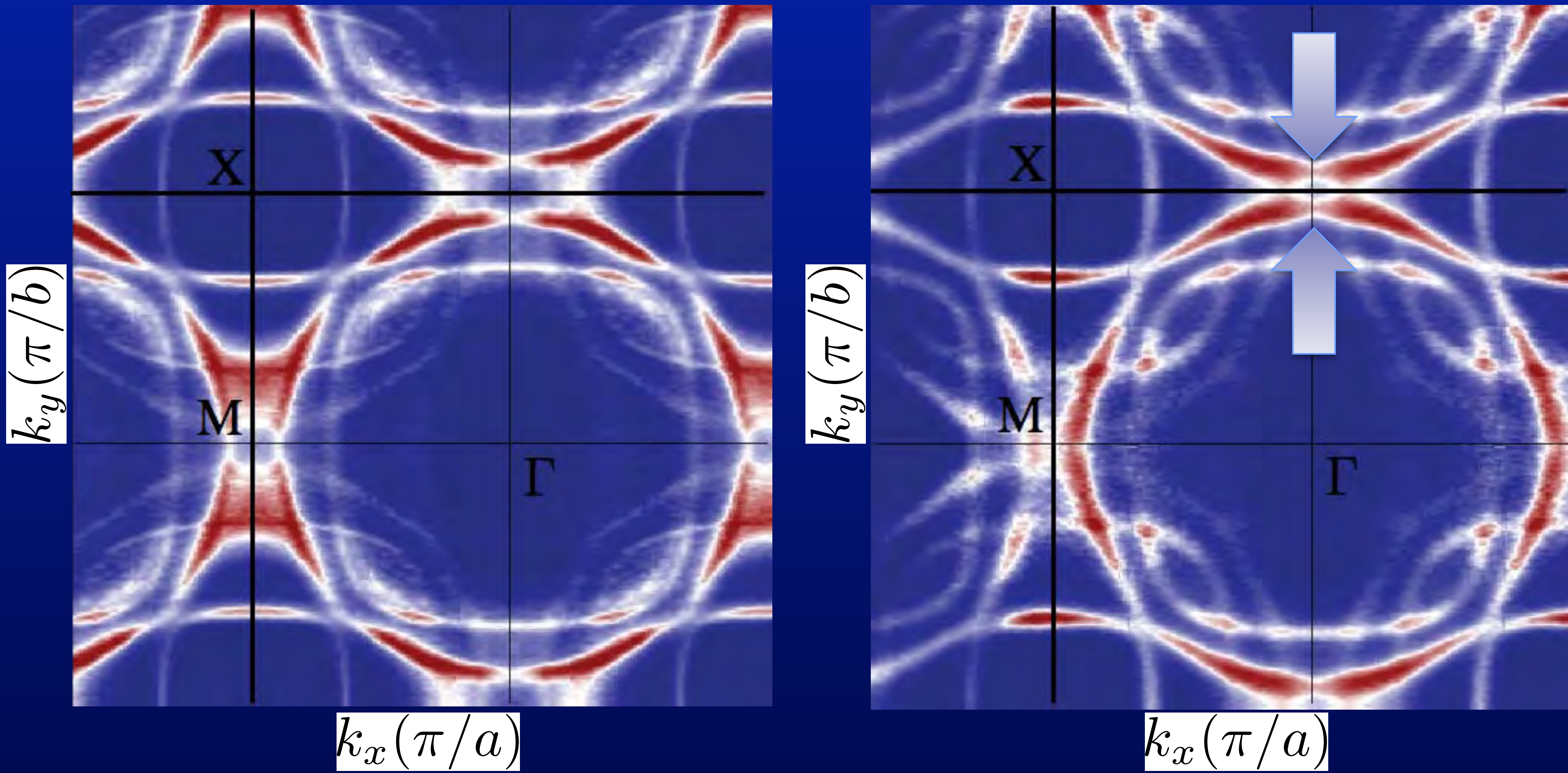
Much Larger Elastic Strains are Possible in Epitaxial Thin Films



In-Plane Lattice Constant (Å)

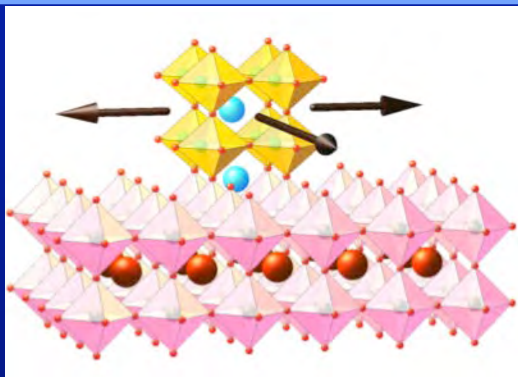
Strain Control of Fermi Surface in Sr_2RuO_4

Unstrained Sr_2RuO_4 | Sr_2RuO_4 on $SrTiO_3$ (+0.9%)

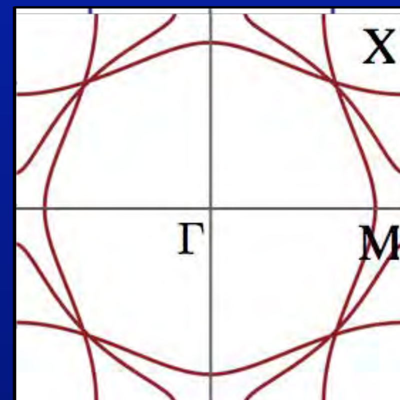


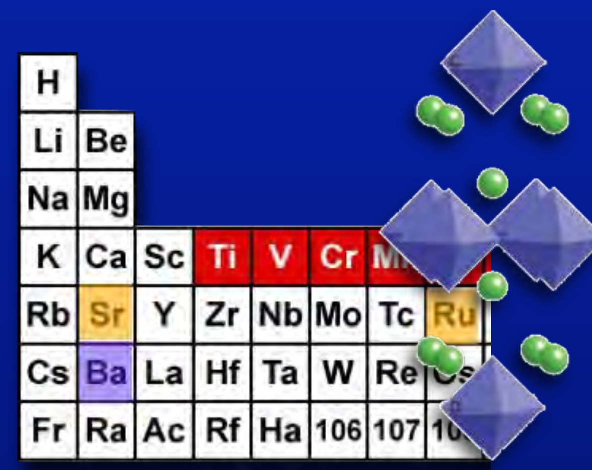
thin films still non-superconducting due to extreme sensitivity of spin-triplet SC to disorder, but low resistivities (5 μΩ·cm)

Pushing to Higher "strains" using Epitaxial Stabilization of Ba_2RuO_4



Lifshitz transition





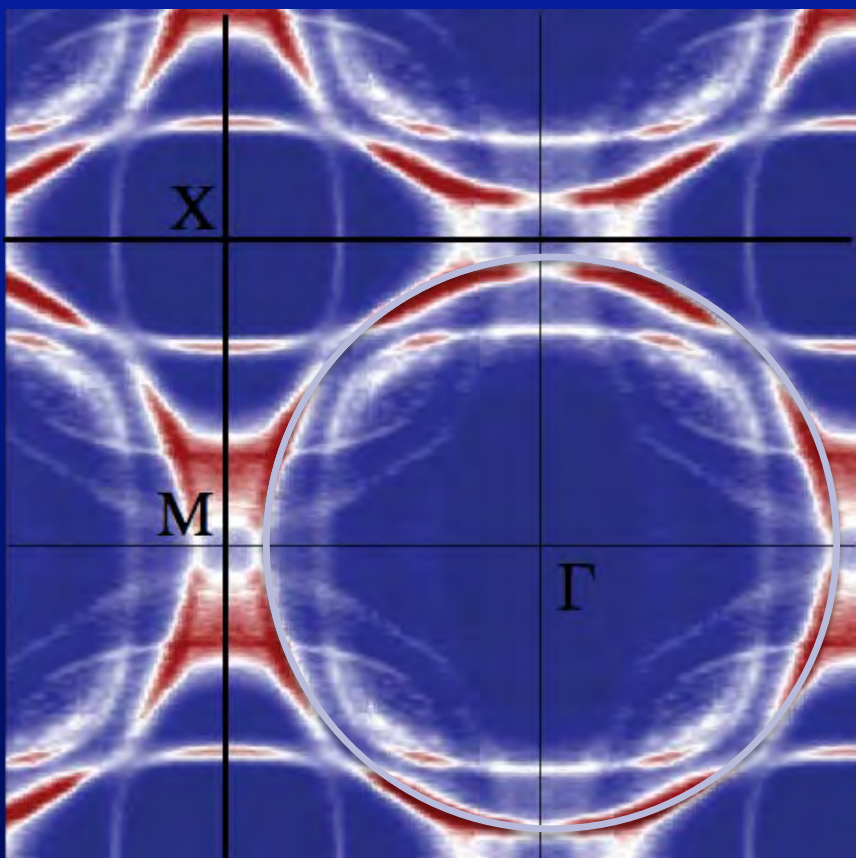
bulk Sr_2RuO_4	bulk Sr_2RuO_4 (uniaxial)	$SrTiO_3$	$DyScO_3$	$GdScO_3$
3.860	3.868 (+0.2%)	3.905 (+0.9%)	3.942 (+2.1%)	3.960 (+2.6%)

In-Plane Lattice Constant (Å)

- Ba_2RuO_4 is isoelectronic and isostructural to Sr_2RuO_4
- Metastable in bulk, but can be epitaxially stabilized

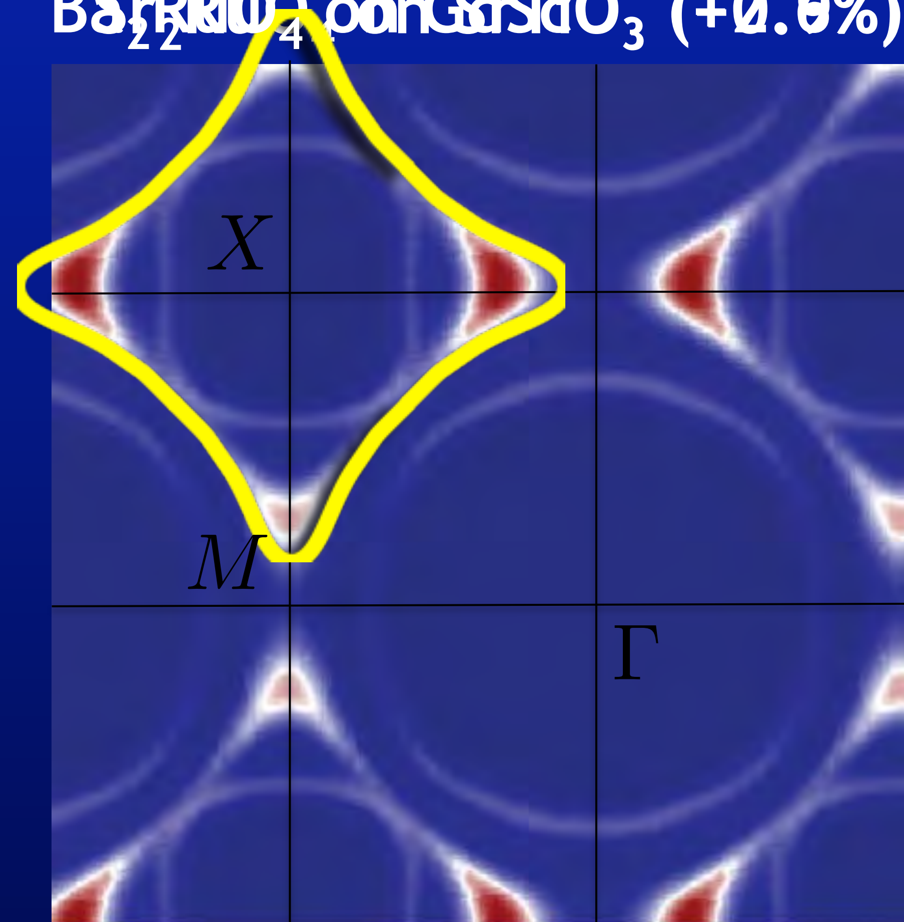
Strain Control of Fermi Surface in Sr_2RuO_4

Unstrained Sr_2RuO_4



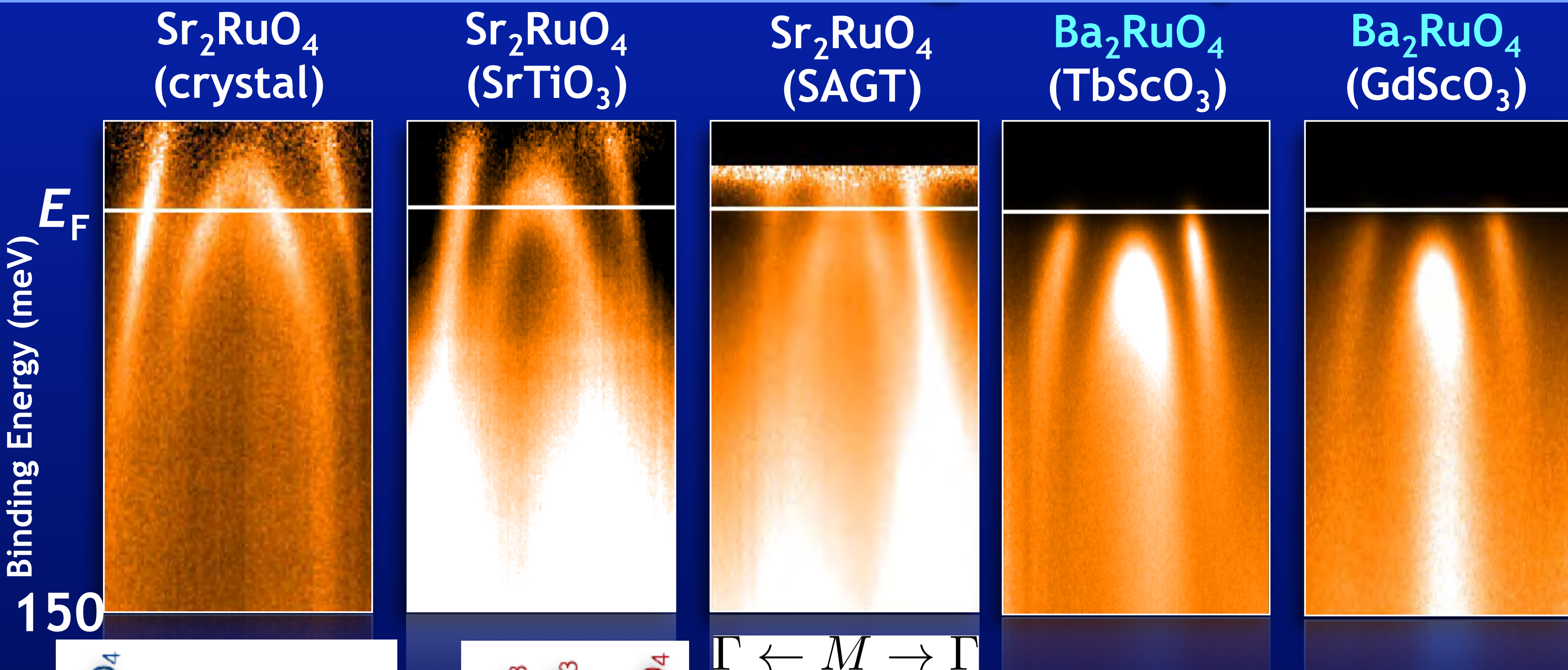
Ba_2RuO_4 on $SrTiO_3$ (+2.0%)

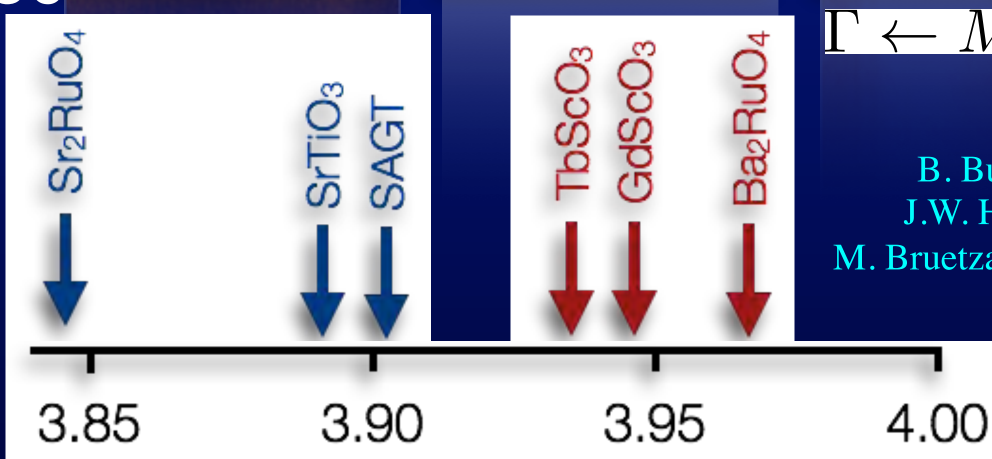
Sr_2RuO_4 on $GdScO_3$ (+0.6%)



Large epitaxial strains turn the large electron-like Fermi surface closed around Γ to a hole-like Fermi surface closed around X

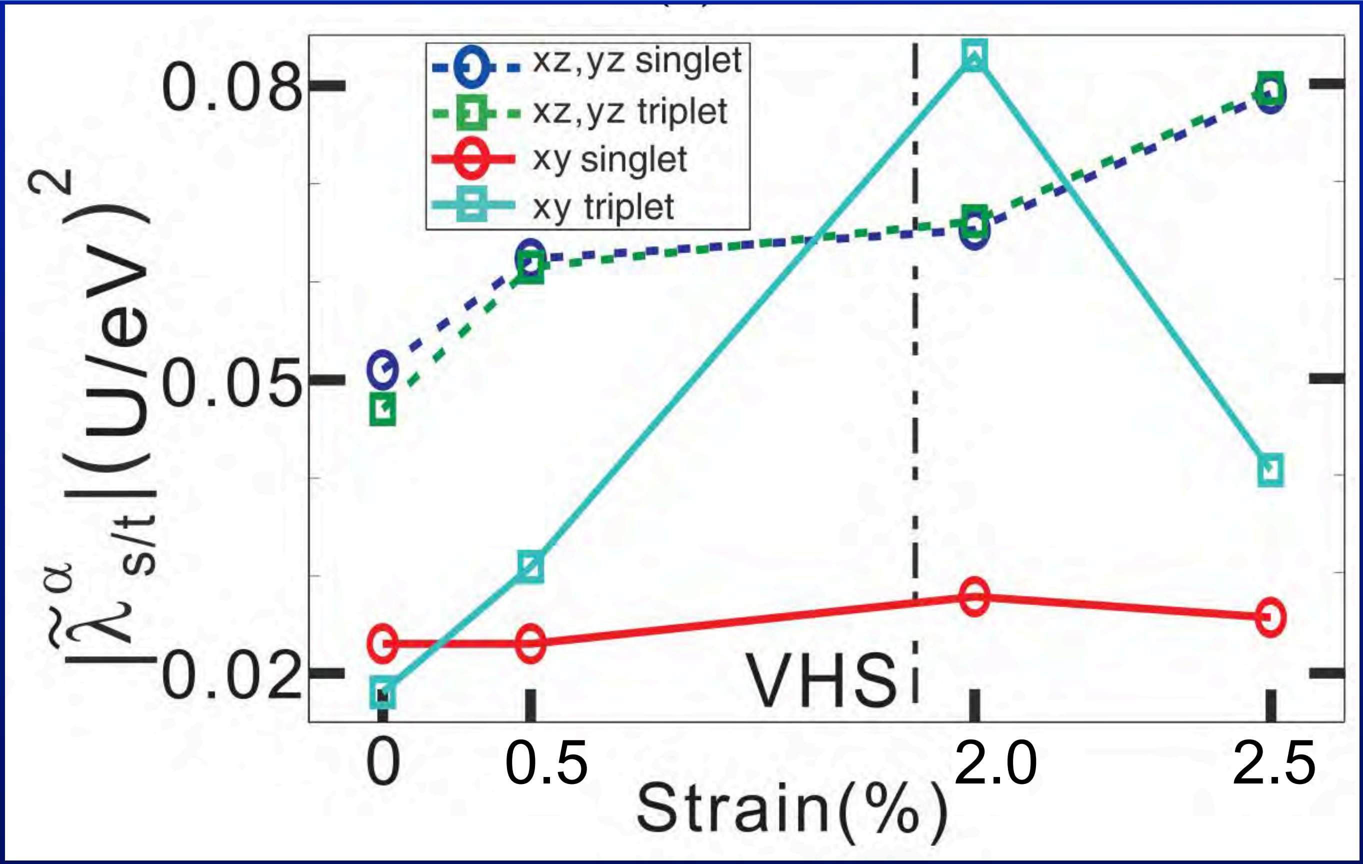
Strain Control of Band Structure and van Hove singularity





B. Burganov, C. Adamo, A. Mulder, M. Uchida, P.D.C. King, J.W. Harter, D.E. Shai, A.S. Gibbs, A.P. Mackenzie, R. Uecker, M. Bruetzam, M.R. Beasley, C.J. Fennie, D.G. Schlom, and K.M. Shen, *Physical Review Letters* **116** (2016) 197003.

Theory Predicts Enhancement of Spin-triplet Superconductivity



Eun-Ah Kim

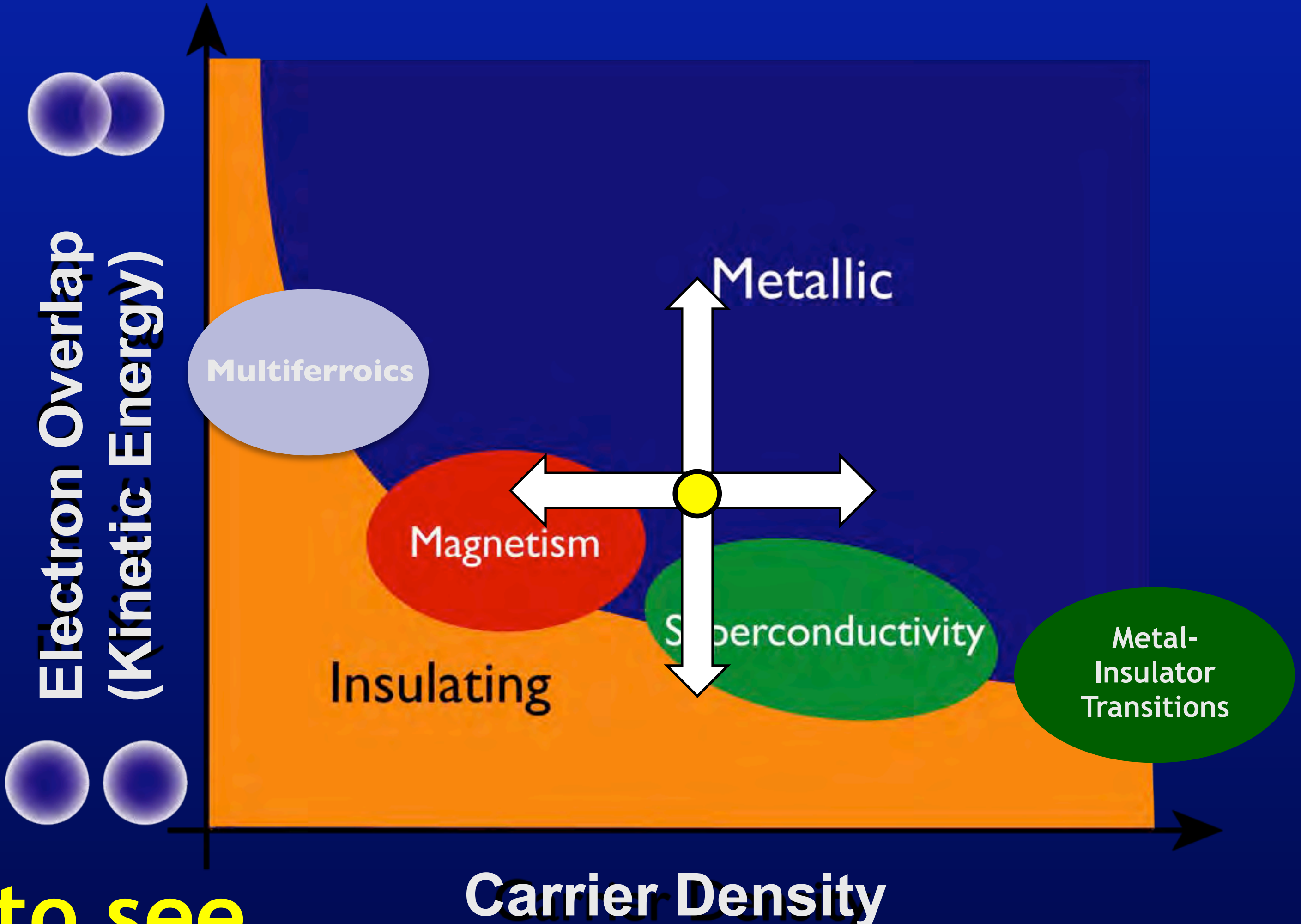
Craig Fennie

Spin-triplet superconductivity is predicted to be strongly enhanced when the van Hove singularity is brought near the Fermi level (see arXiv:1604.06661)

Imagine Tuning Quantum Materials

Independent Control of

- Strain
- Doping
- Octahedral Rotations
- Proximity Effects
- Dimensionality
- …



With ability to see changes in electronic structure

Rules for QM Synthesis

- Gibbs' Rule
  $\Delta G < 0$ to form stable phases

- Matthias's Rules for Superconductors
  … "Stay away from Theorists"

- Pauling's Rules for Crystal Structures
  Radius ratio criteria for stability

BREAK THE RULES!

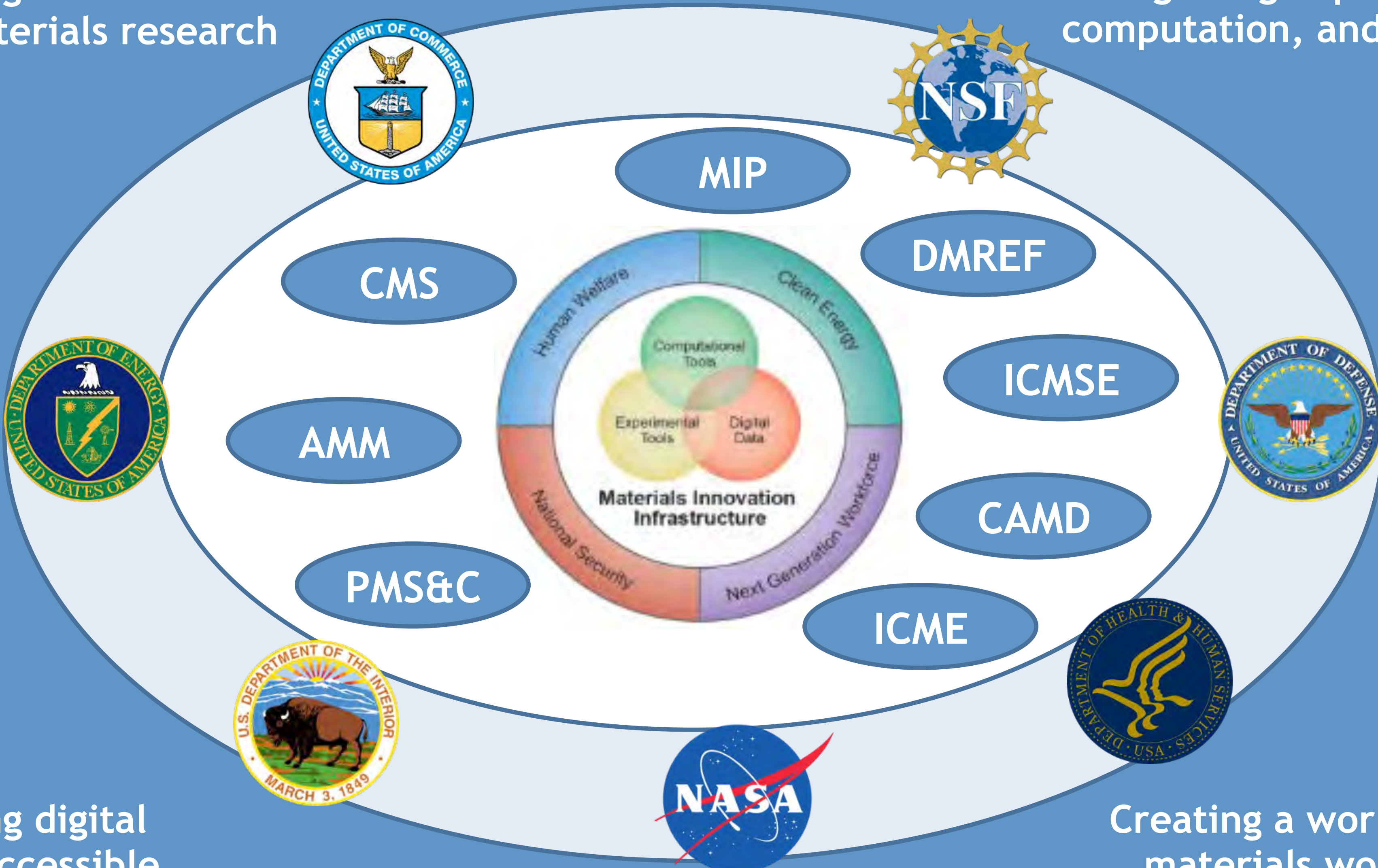
My Four Requests

- Please do *not* Pollute the Literature with Predictions on Impossible Materials
- Please *do* Consider the Limits of Synthesis
- Please *do* use the new NSF-MIP National User Facilities (PARADIM + 2DCC)

Materials Genome Initiative

Leading a culture shift in materials research

Integrating experiment, computation, and theory



Making digital data accessible

Creating a world-class materials workforce

Credit: Chuck Ward (AFRL)

Enabling the discovery, development, manufacturing, and deployment of advanced materials at least twice as fast as possible today, at a fraction of the cost.

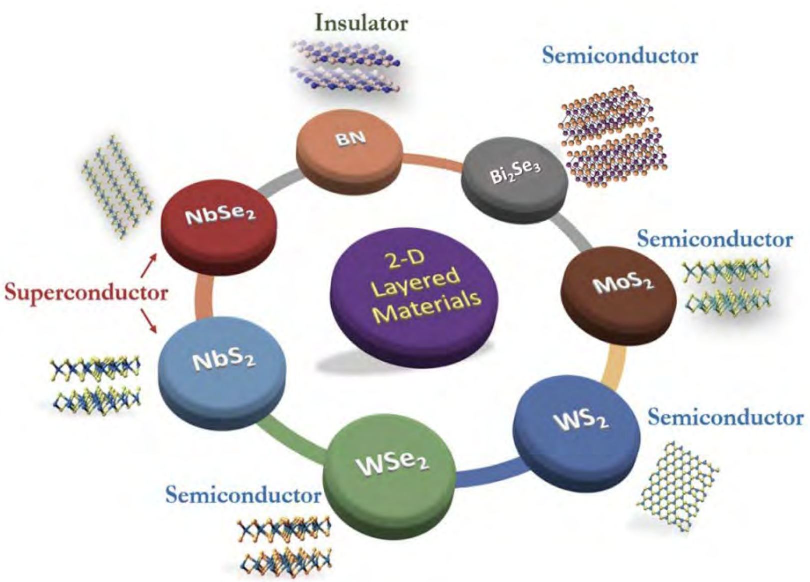
2D Crystal Consortium

NSF Materials Innovation Platform

PennState

Broad access to compelling synthetic tools with integrated theory support

2D chalcogenide monolayers, surfaces and interfaces are emerging as a compelling class of systems with transformative new science that can be harnessed for novel device technologies in next-generation electronics.



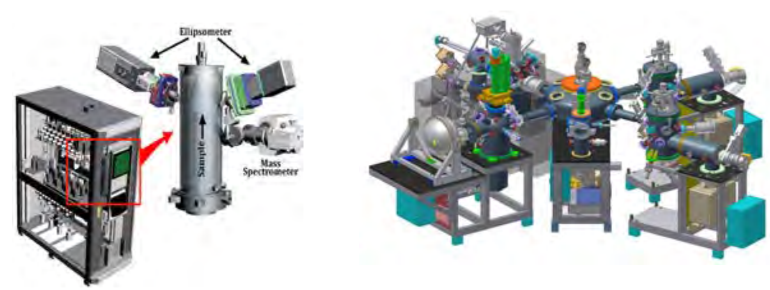
Hybrid MBE
Chalcogenide MOCVD
CVT, Bridgman

in situ measurement | *insights into growth*

STM/AFM
ARPES
4-probe
Raman, PL

characterization & interpretation

DFT
Reactive FF
Monte Carlo
Phase field



An NSF **user facility** with broad access:

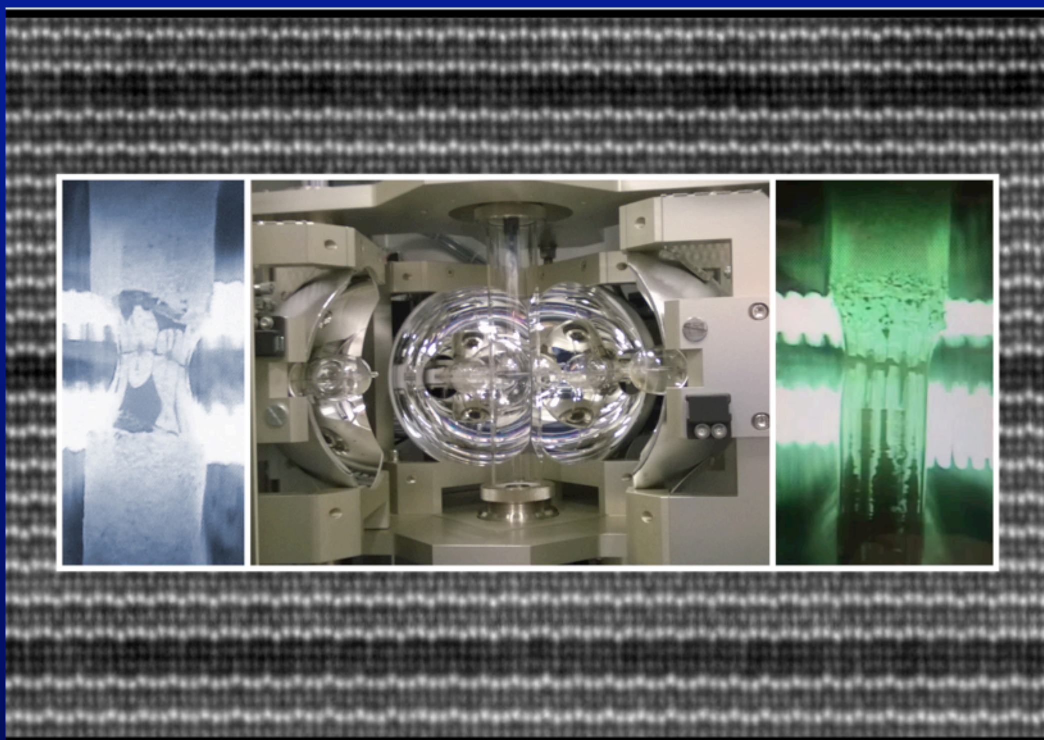
- Open calls for user proposals,
- No user fees for academic use
- Access to a team of local experts
- Community knowledge-base of synthetic protocols

- Webinars, Workshops, Website resources
- Partnership opportunities with PUI, MSI

mip.psu.edu

PARADIM

PLATFORM FOR THE ACCELERATED REALIZATION, ANALYSIS & DISCOVERY OF INTERFACE MATERIALS



New $25 Million National User Facility to help YOU

BREAK THE RULES!

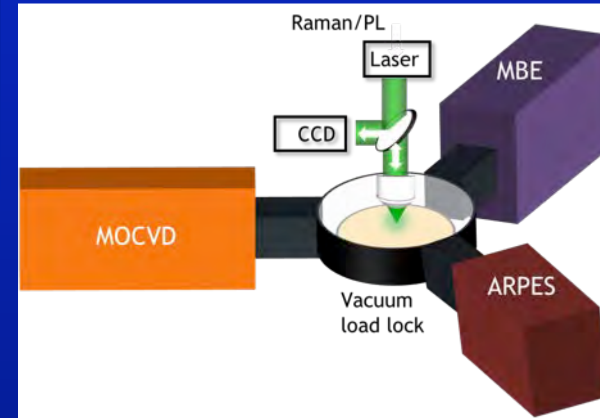
for FREE

www.paradim.org

PARADIM

User Facilities

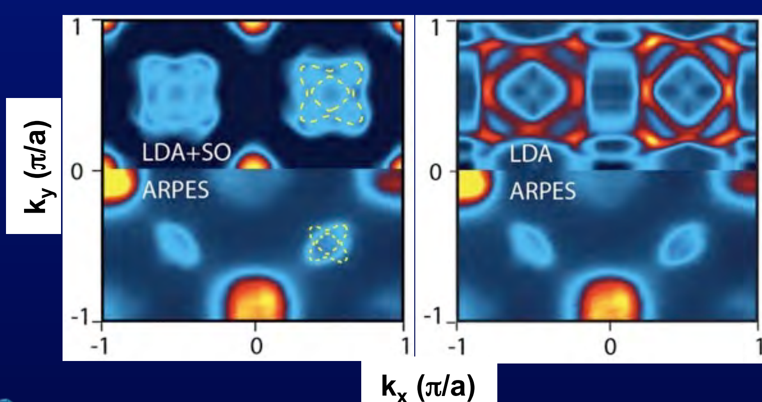
Bulk



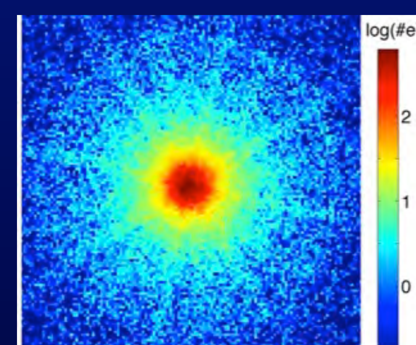
Thin Film

New Chemistry
New Physics
New Materials Science
New Materials

Theory & Computation



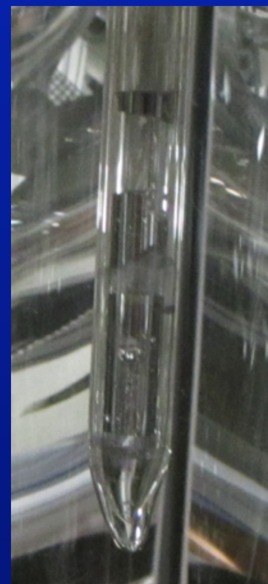
Electron Microscopy
Characterization



PARADIM

Bulk Crystal Growth User Facility

Expanded Growth Conditions



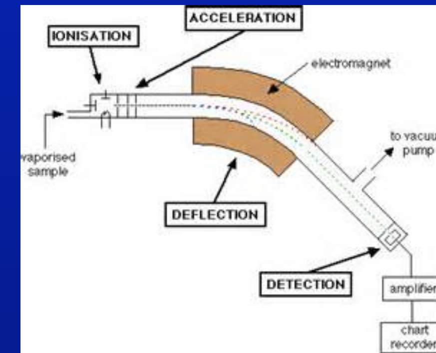
P = 300 atm (first in world)
Supercritical fluids

Safe highly toxics,
Bridgeman in FZ
(first $FeSc_2S_4$ crystals)

Routine, *in situ* Growth Guidance

X-ray CT and Laue

Identify origin of
defect structures



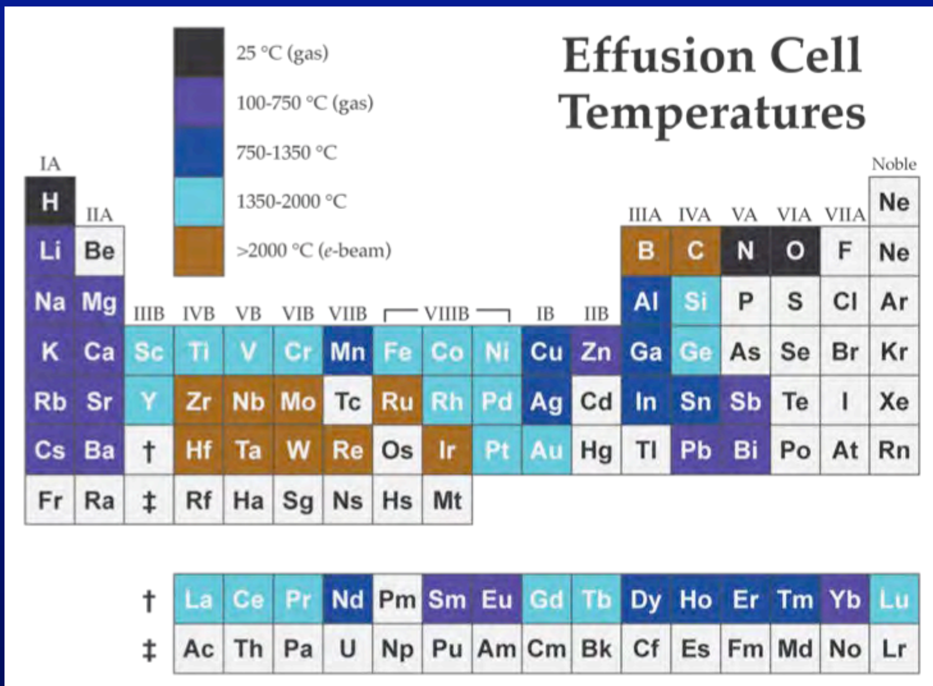
Vapor Equilibria

Tyrel McQueen

Thin Film User Facility (opens 2017)

Expanded Growth Conditions

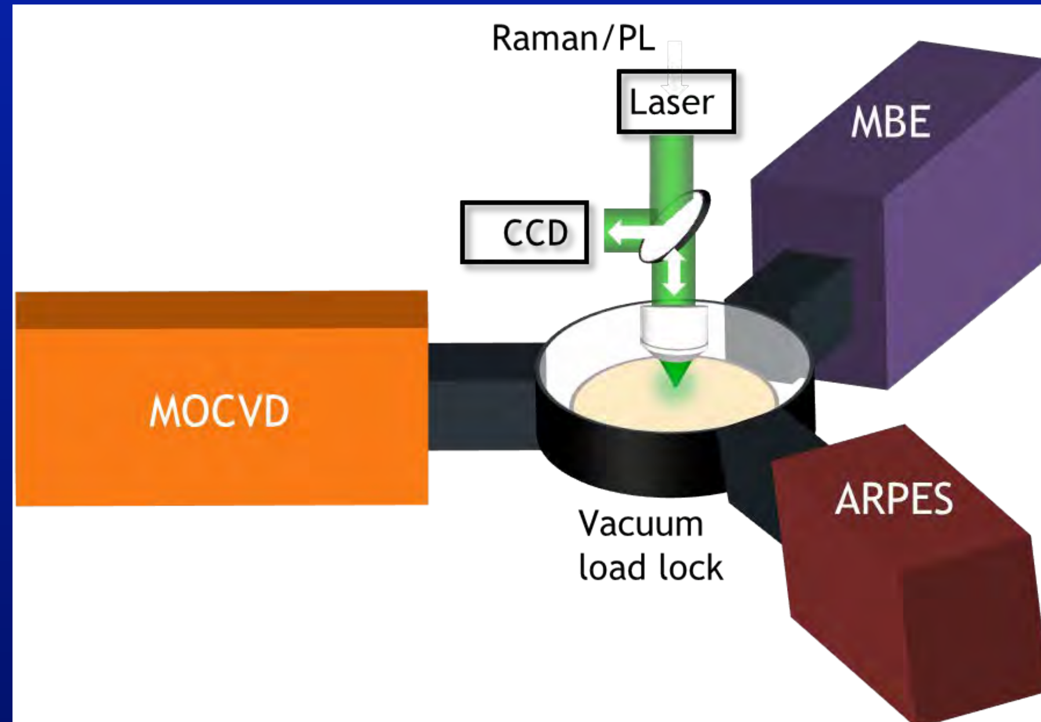
Any 11 of **62 elements** by MBE at one time
(and refills without breaking chamber vacuum)
$T_{sub} < 1400$ °C
Many others (e.g., chalcogenides) via MOCVD



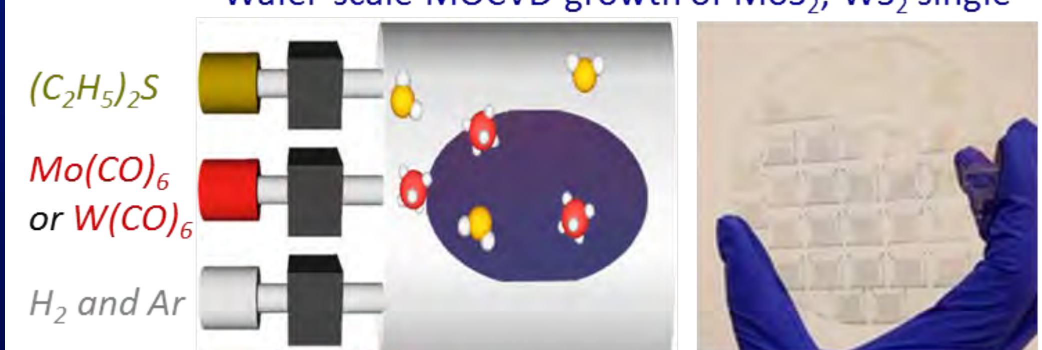
Jiwoong Park

PARADIM

Routine, *in situ* Growth and Characterization



Wafer-scale MOCVD growth of MoS_2, WS_2 single



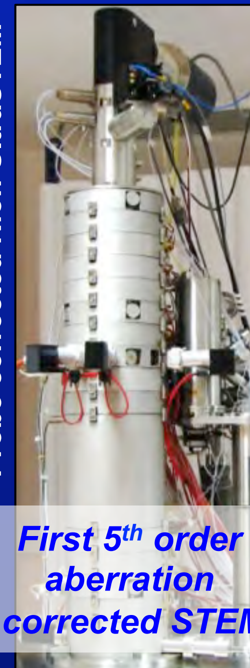
Muller, **Park**, *Nature* **520** (2015) 656.

Electron Microscopy User Facility

FEI T12 TEM

FEI F20 monochromated S/TEM

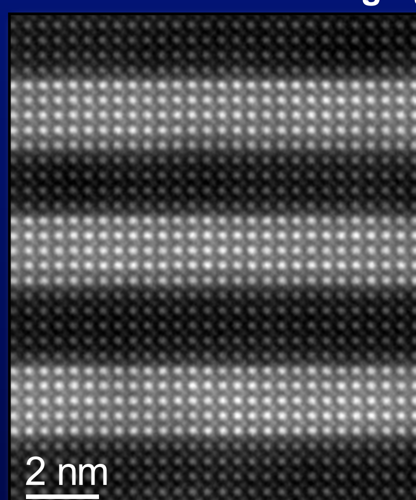
Probe corrected Nion UltraSTEM



Probe Corrected FEI Titan Themis cryoSTEM

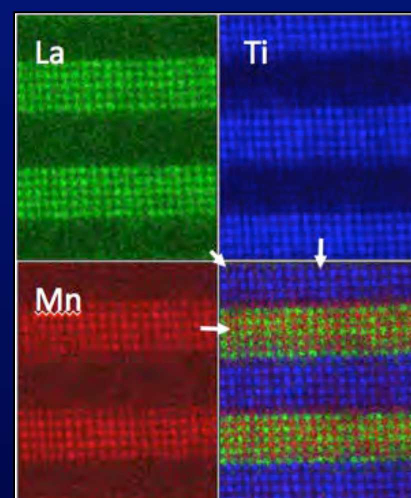
Imaging grains in 2D materials

Atomic resolution Imaging



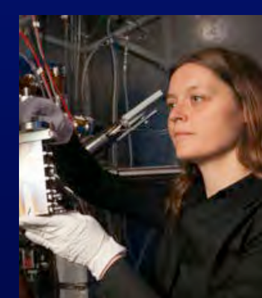
Kourkoutis, Song, Hwang, Muller, *PNAS* **107** (2010) 11682

Atomic resolution Elemental Mapping



Muller, Kourkoutis, Murfitt, Song, Hwang, Silcox, Dellby, Krivanek, *Science* **319** (2008) 1073

- **Atomic resolution imaging + spectroscopic mapping at LN_2 temp.**
- **Magnetic imaging by Lorentz TEM**



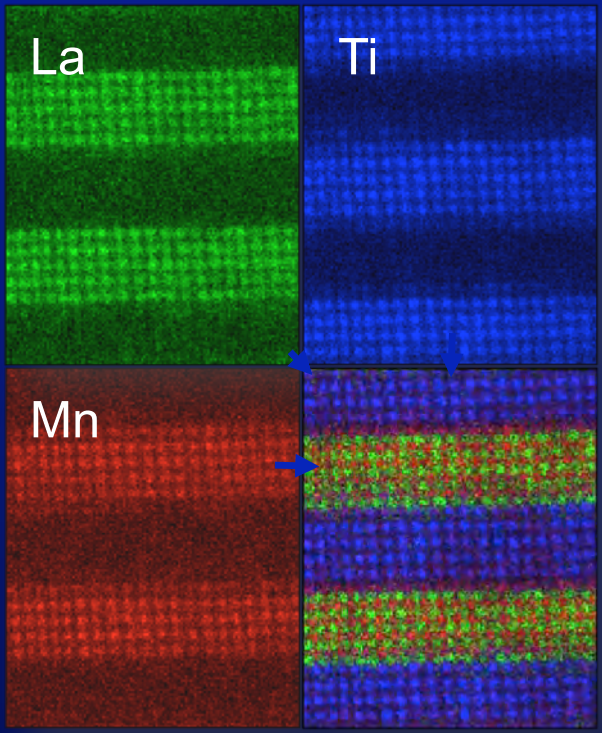
Lena Kourkoutis

PARADIM

Electron Microscopy for Materials Characterization at the Atomic Scale

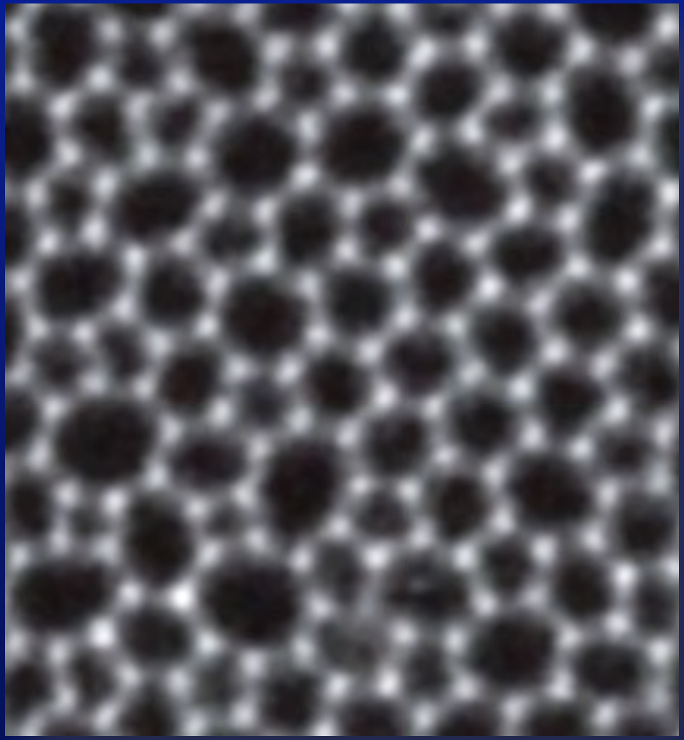
Tools for:

Chemical Imaging



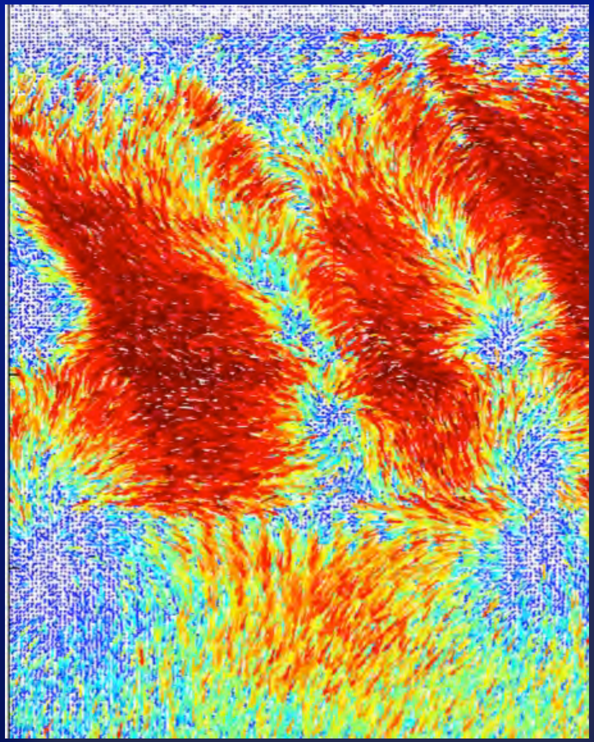
Science **319**, 1073 (2008).

Seeing Every Atom



Nano Lett. **12**, 1081 (2012)

Physical Properties



Microsc. and Microanal. **22**, 237 (2016)

PARADIM

NSF

Theory User Facility

Helping to close the gap with experiment

Two modes of operation

Consultation—Advise and Help

Key elements:

- *Fundamental theory*
- *Well-known Algorithms*
- *Software packages*
- *Efficiency techniques*

Aided by: Materials-by-Design Toolbox

- *Community*
- *On-Line Short Courses*
- *Open-source code*
- *Databases*
- *Tutorials*
- *Written instructions*

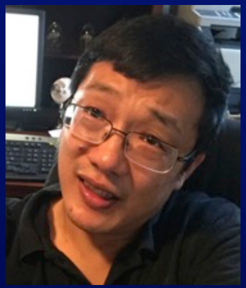
Collaboration—coauthoring

Key elements:

- *Advanced/new theory*
- *Advanced/new Algorithms*
- *Specialty Software packages*
- *Runtime optimization*

Aided by: Materials-by-Design Toolbox

- *Community*
- *Databases*
- *Commercial codes*
- *Specialized codes*
- *Code modifications*

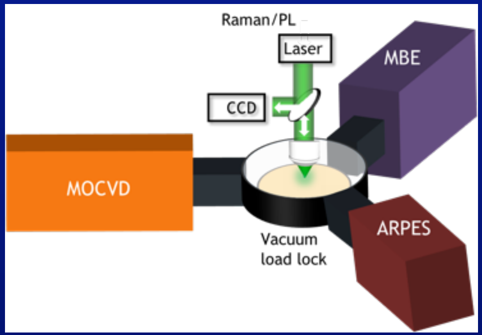


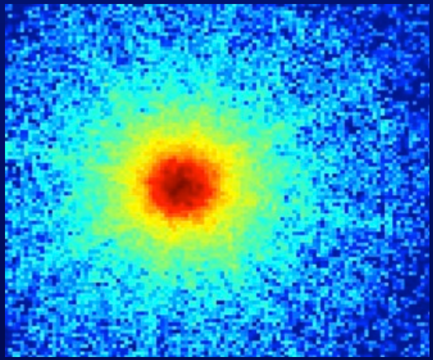
Larry Wang

PARADIM

PARADIM — A National User Facility

- Theory to help guide experiment
- High-pressure (supercritical fluid) floating-zone growth
- Mass spectrometry and computed tomography *during* bulk crystal growth
- Integrated MOCVD + MBE + ARPES
- High sensitivity, high dynamic range pixel array detector for quantitative mapping of ***E*** and ***B*** fields with sub-nm resolution
- Stable cryo-stages for STEM and STEM-EELS at 20 K and 80-1200 K





FREE to the academic community via 2-page proposals

Summer Schools to build a community of practitioners

Electron Microscopy, June 18th-23th, 2017

Crystal Growth and Design, July 16th-21th, 2017

PARADIM

http://paradim.cornell.edu

NSF

My Four Requests

- Please do *not* Pollute the Literature with Predictions on Impossible Materials
- Please *do* Consider the Limits of Synthesis
- Please *do* use the new NSF-MIP National User Facilities (PARADIM + 2DCC)
- Please *do* Tell me First if you Predict a Materials-Specific Embodiment of a Room-Temperature Superconductor