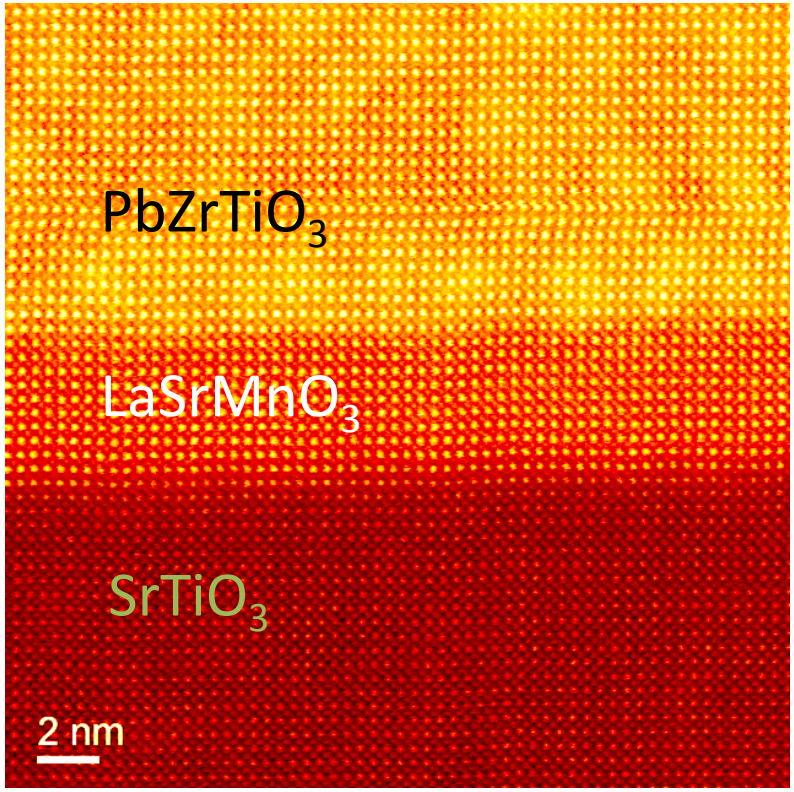
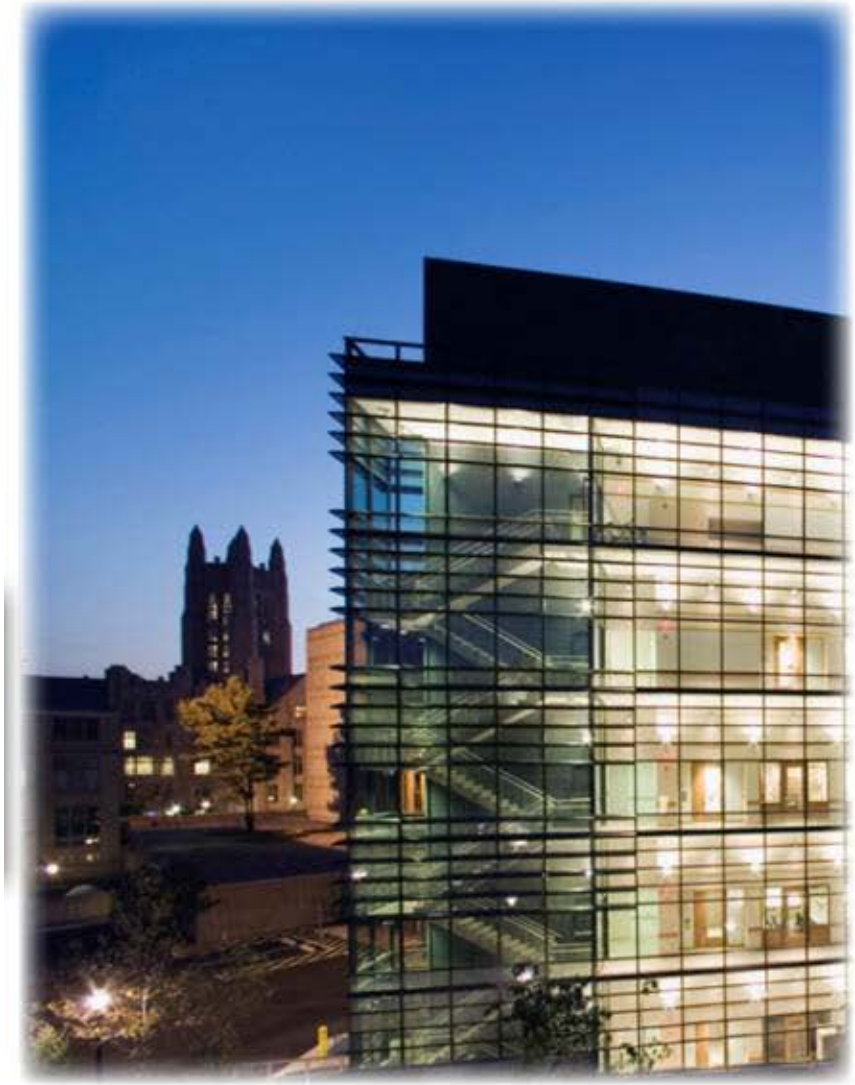
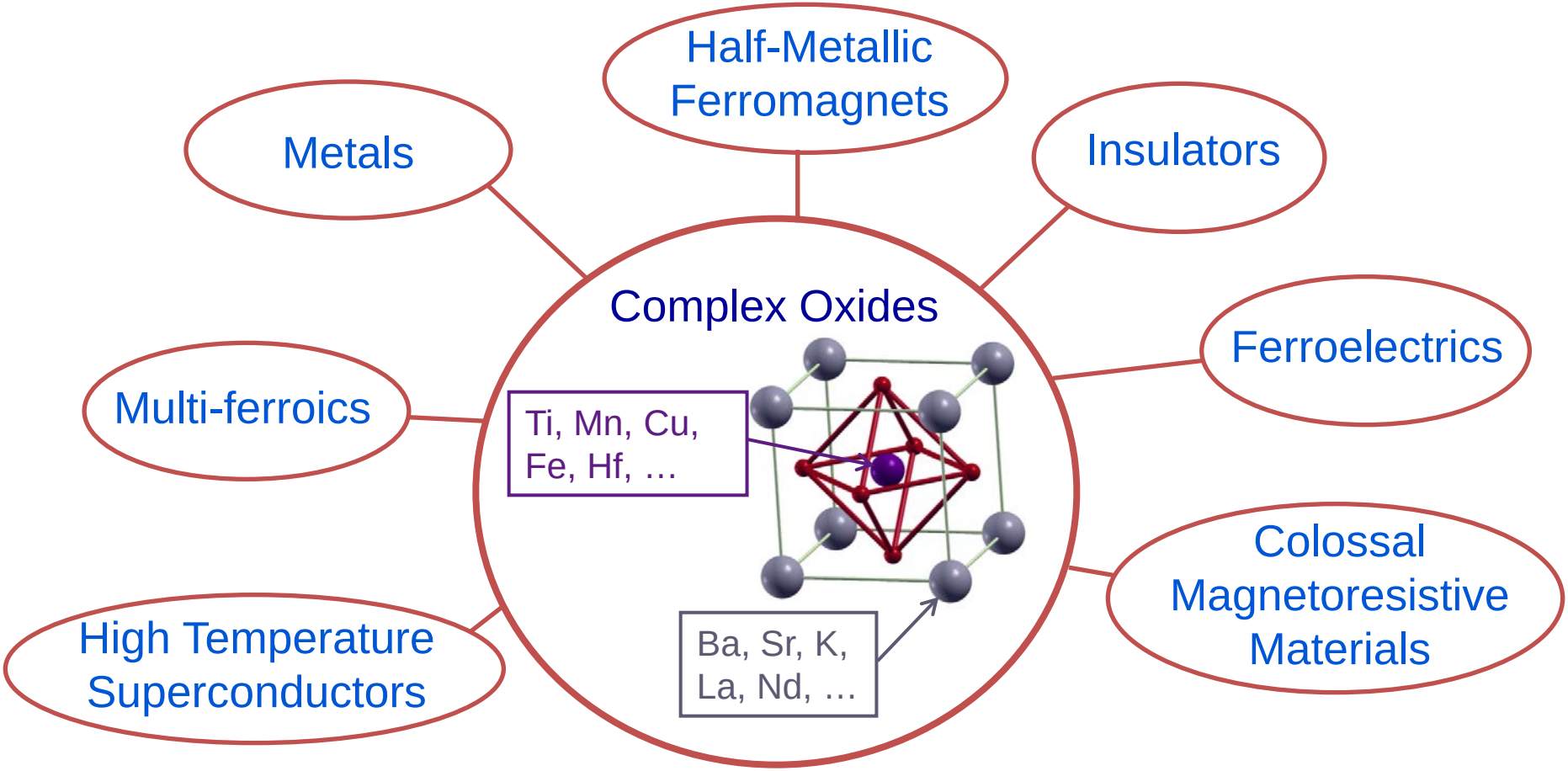
Center for Research on Innovative Structures and Phenomena

Southern Connecticut State University

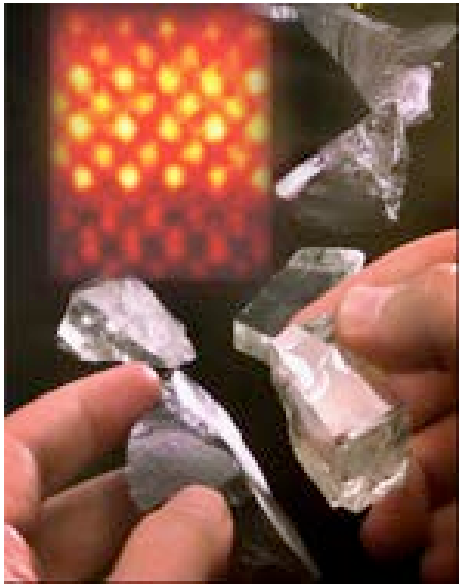




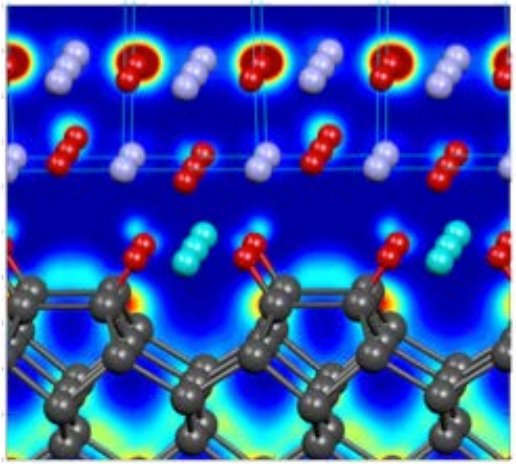
Complex Oxides: Rich in Phenomena



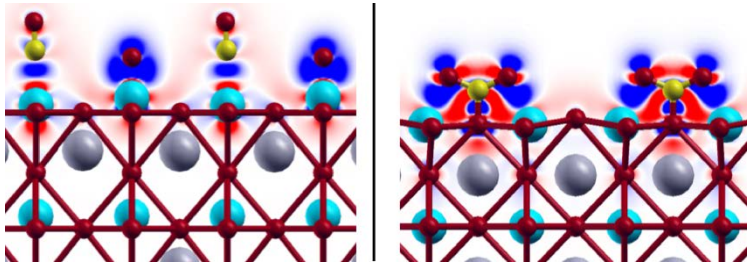
Complex Oxides at the Atomic Scale



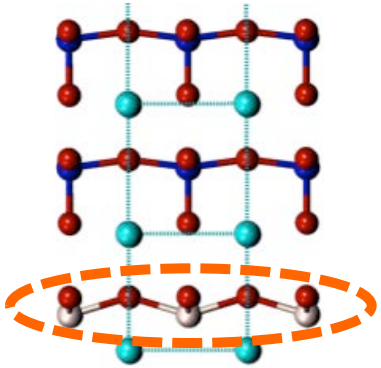
What happens when two materials are put together with atomic precision?



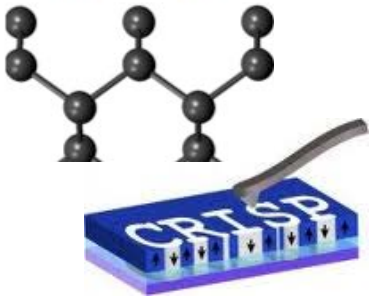
Design
Control
Characterize



Control chemistry or growth at surfaces?



Can we *design* novel interfaces & surfaces?



Precisely *characterize* surfaces or interfaces?

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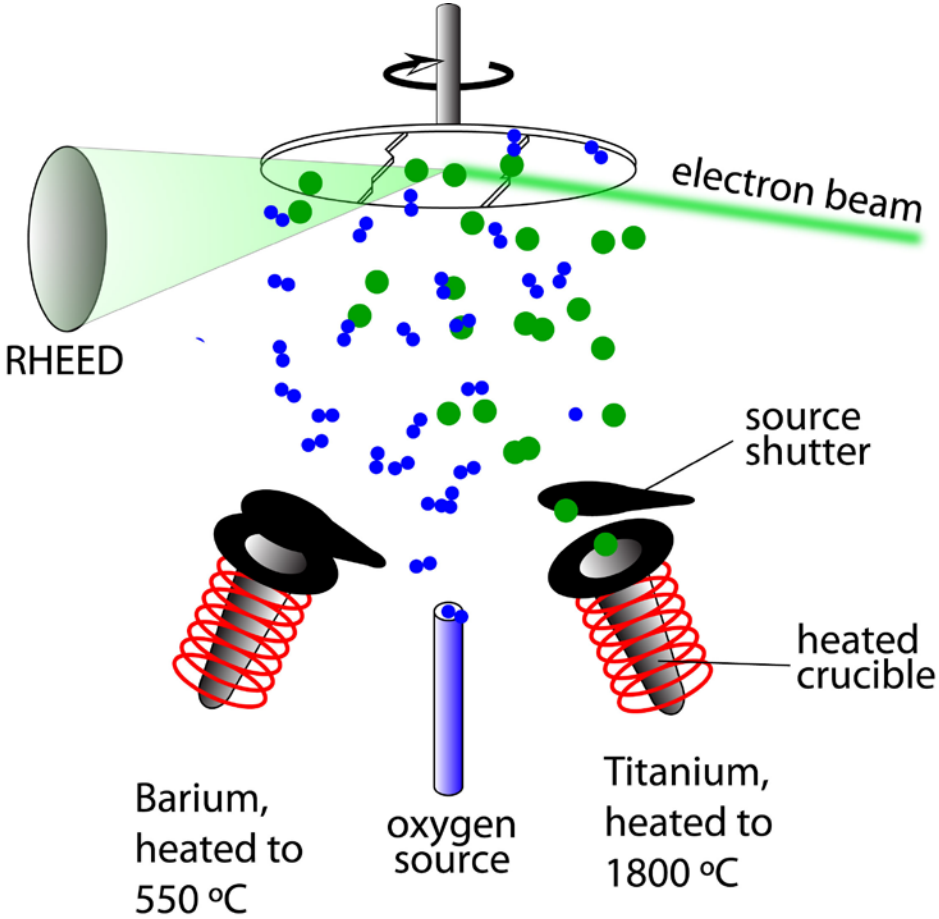
Engines of atomic layer control – Molecular Beam Eptiaxy

- UHV chamber
- Heated metal sources
- Heated substrate
- In-situ diffraction
  - Surface sensitivity
- Atomic layer control



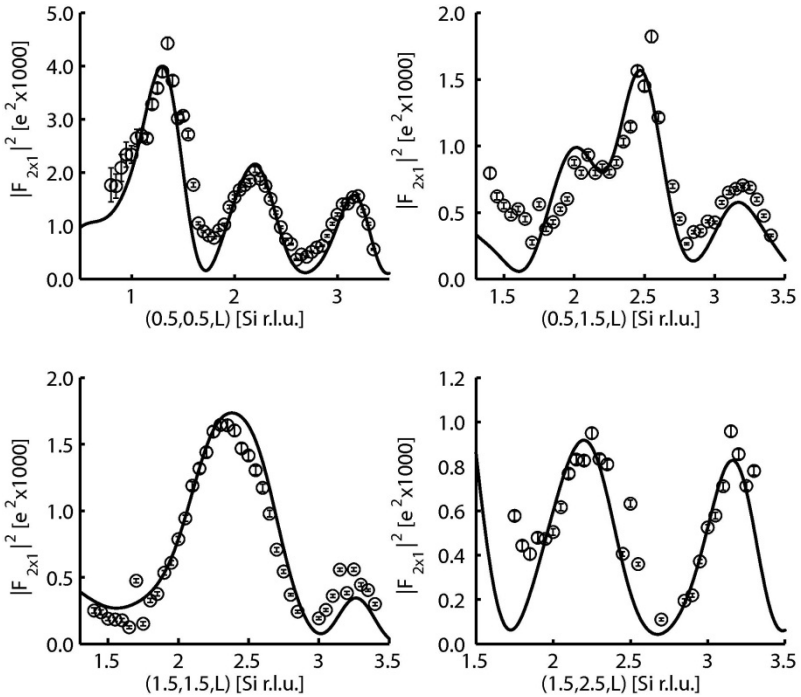
Complex-oxide community

- Groups funded by NSF Materials Research Science and Engineering Centers (MRSEC) program
- ~$1M/year for 3-6 years.
- Thin film oxide growth.
  - PLD
  - MBE
  - Sputtering

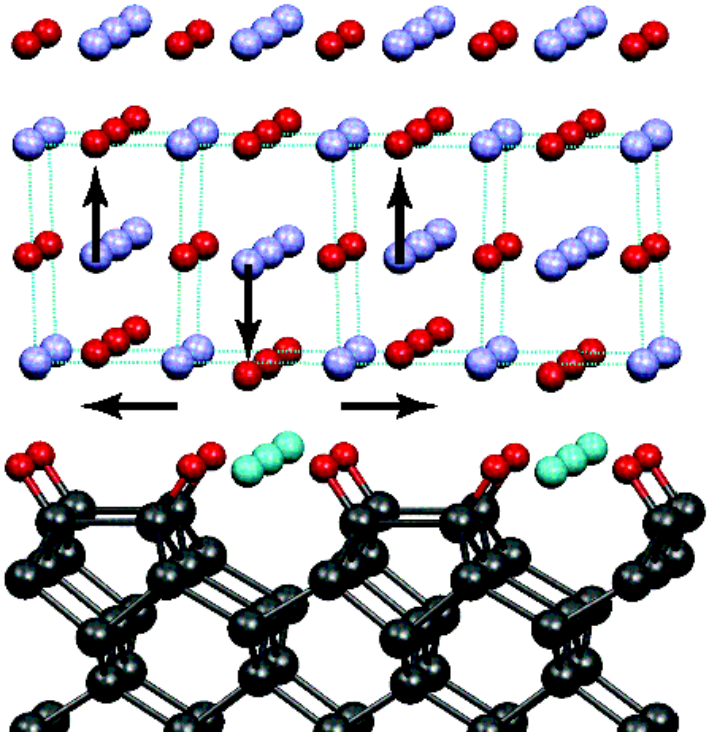
- Cornell
- UC Santa Barbara
- Ohio State University
- Penn State University
- The University of Texas, Austin (MIRT)
- *Yale*
- University of Nebraska

Synchrotron X-rays

X-ray scattering from *interfaces*



x-ray scattering from 2x1 symmetry at BaO/Si interface



- Joint experiment / theory approach
- Delivers < 0.1 Å accuracy

Argonne NATIONAL LABORATORY

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Segal, Reiner, Kolpak, Zhang, **Ismail-Beigi, Ahn, Walker**, *Phys. Rev. Lett*. (2009)
Kolpak, **Walker**, Reiner, Segal, Su, Sawicki, **Broadbridge**, Zhang, Zhu, **Ahn, Ismail-Beigi**, *Phys. Rev. Lett.* (2010)

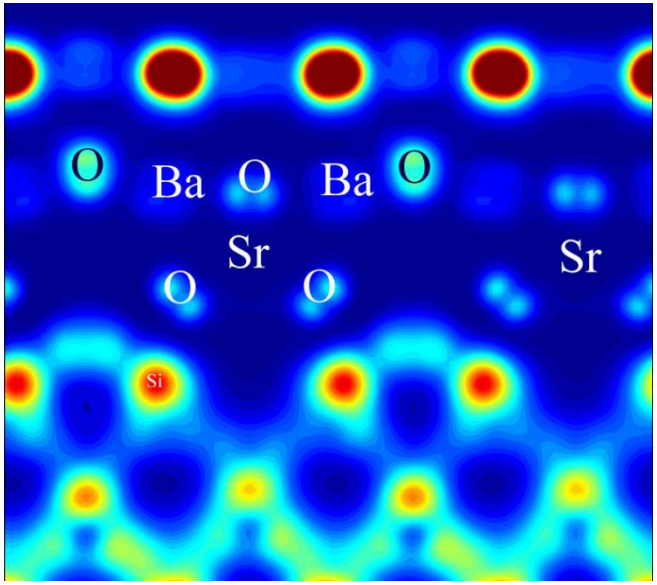
CRISP

Use DFT to zoom in on interface

First bulk-like oxide layer

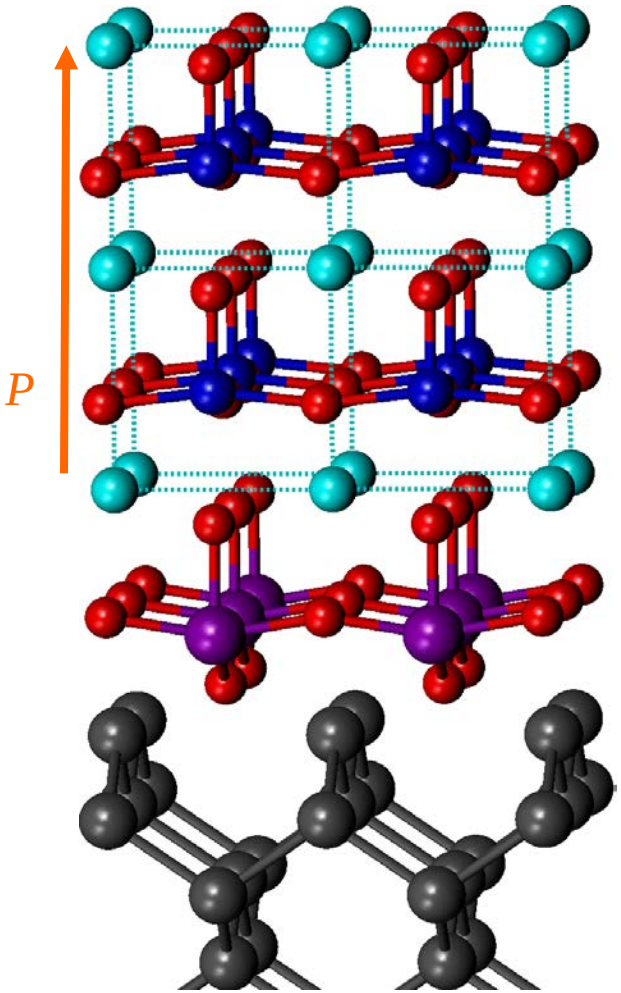
Interface

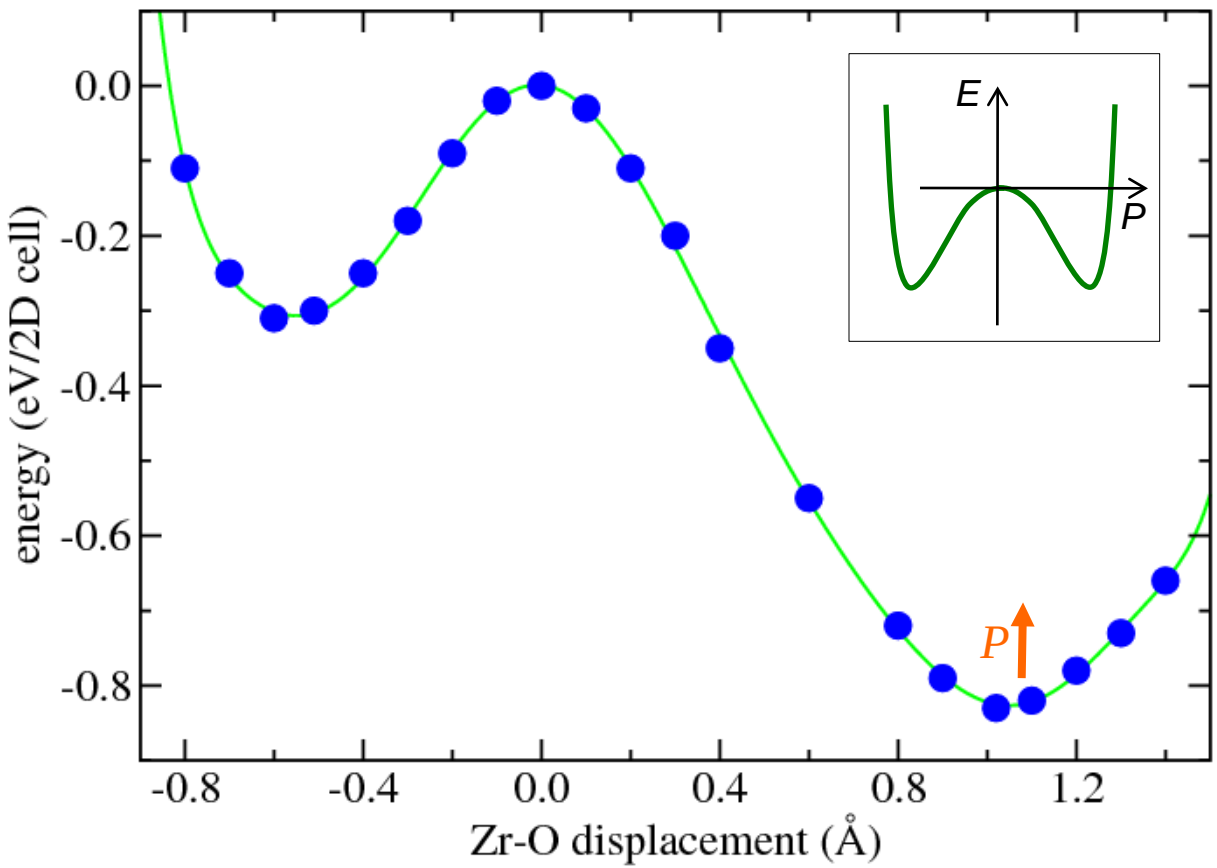
First bulk-like silicon layer



- *We've understood the BaO Si interface -starting interface.*
- *Currently, we are trying to manipulate complex oxide-semiconductor interfaces.*

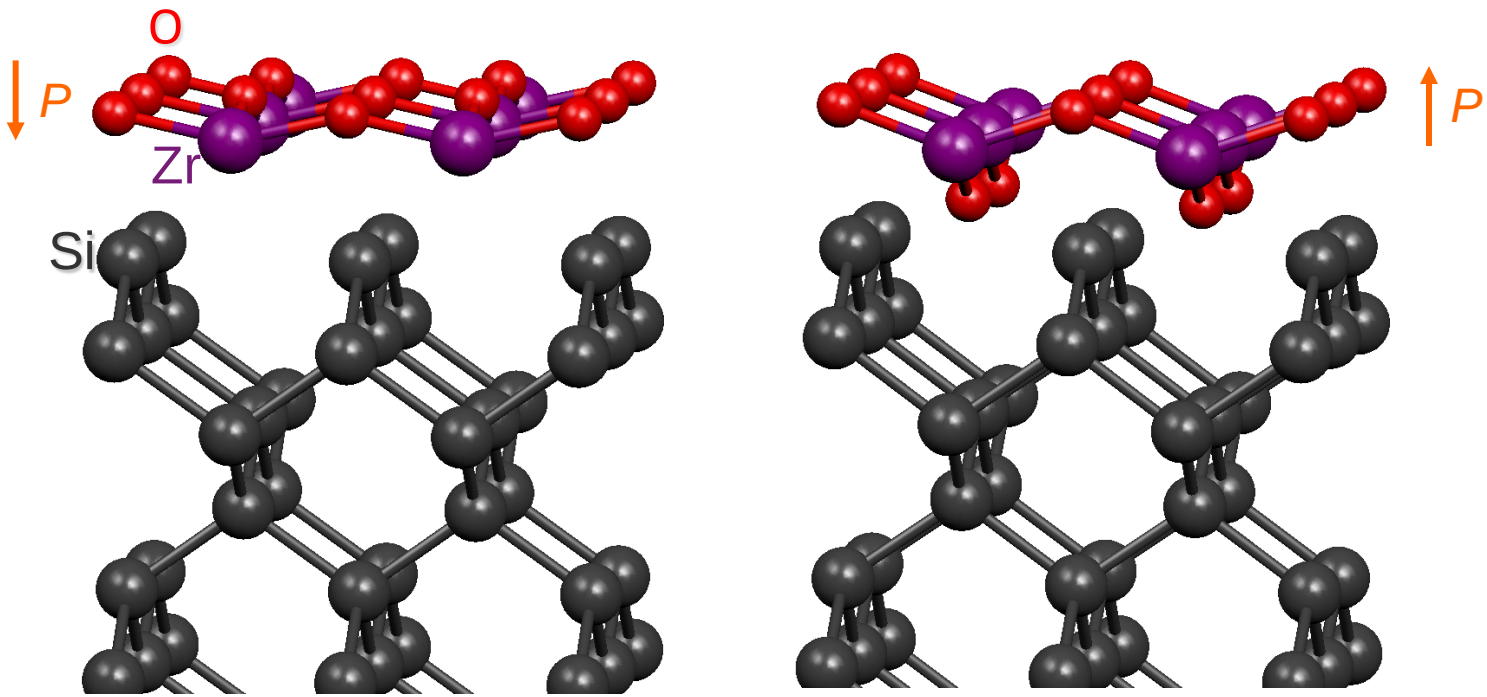
Ferroelectric interfaces $Si/ZrO_2/SrTiO_3$





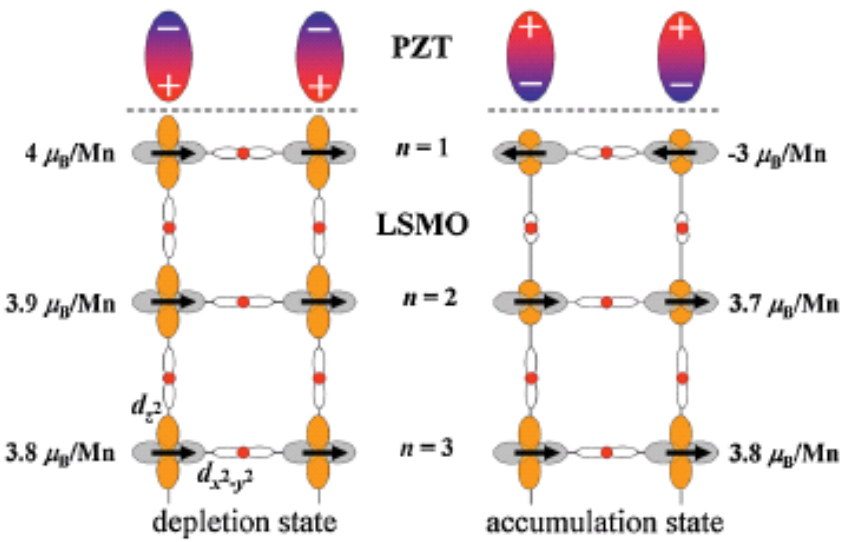
Two stable states with
opposite interface dipoles

Ferroelectric ZrO_2 on Si Surface

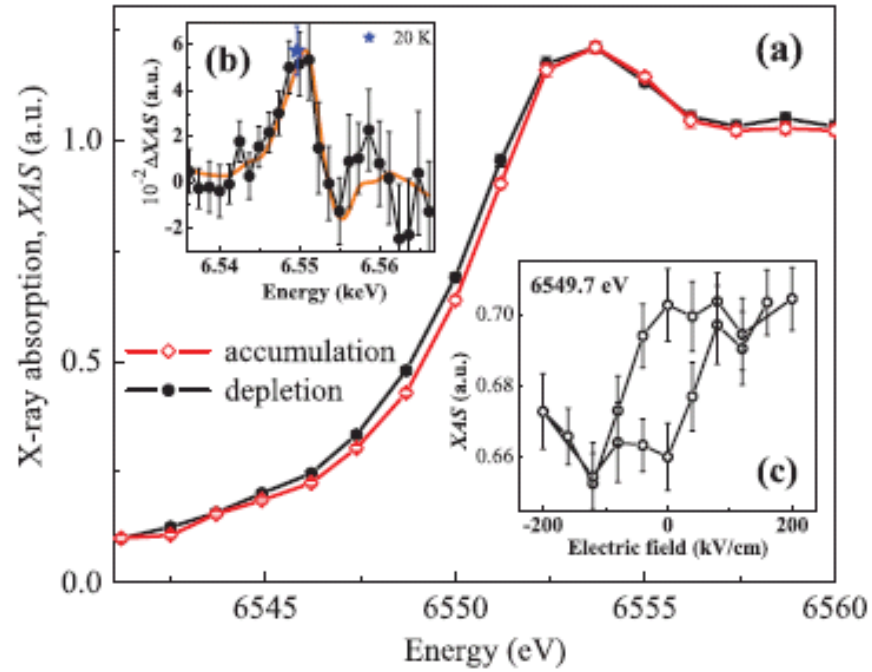


- Monolayers are ferroelectric without a capping oxide
- Change of transition metal valence could lead to catalytic properties
- Allows for surface science observations and manipulations
- Relevance for industry: *can we synthesize this interface with ALD?*

In situ device measurement using a tunable source



Device



Near edge structure

IRG-2: Correlated Electronics

Grand Challenge

Science of the unique properties of complex oxide heterostructures
→ towards enabling new technologies

IRG Members	Role/Expertise
Susanne Stemmer (IRG co-leader)	MBE growth & microscopy
Chris Van de Walle (IRG co-leader)	Theory/defects and interfaces
Jim Allen	Optical/magnetotransport, devices
Leon Balents	Theory/strong electron correlations
Michael Chabinyc	Electrolyte gating
Ram Seshadri	X-ray & neutron diffraction, magnetism
Dmitri Strukov	Devices, circuits

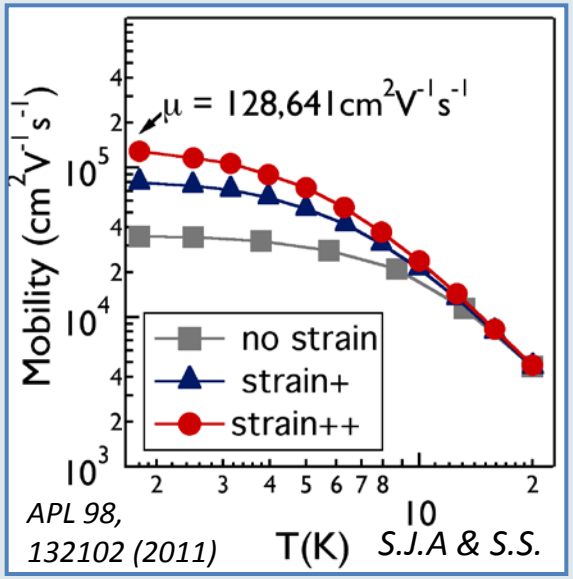
IRG Affiliate	
Anand Bhattacharya (Argonne)	MBE growth

Key to Progress: Near-Perfect Materials

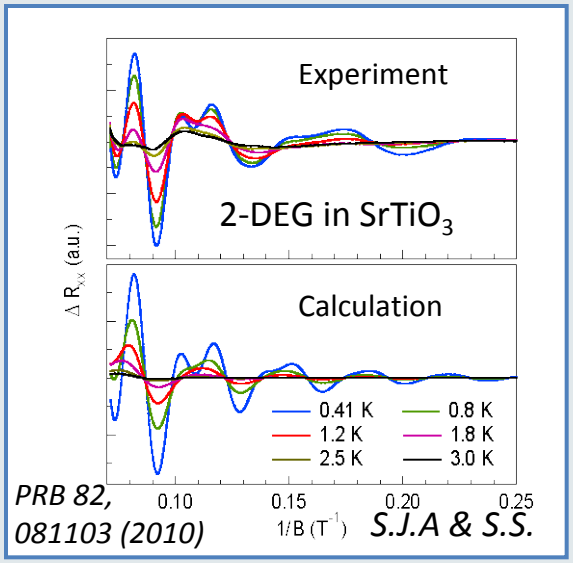
Oxide Molecular Beam Epitaxy

- High-purity , titanium tetraisopropoxide, $Ti(OC_3H_7)_4$
- Low-energetic deposition
- Monolayer control
- Electronic device quality materials

Nature Mater. 9, 482 (2010).



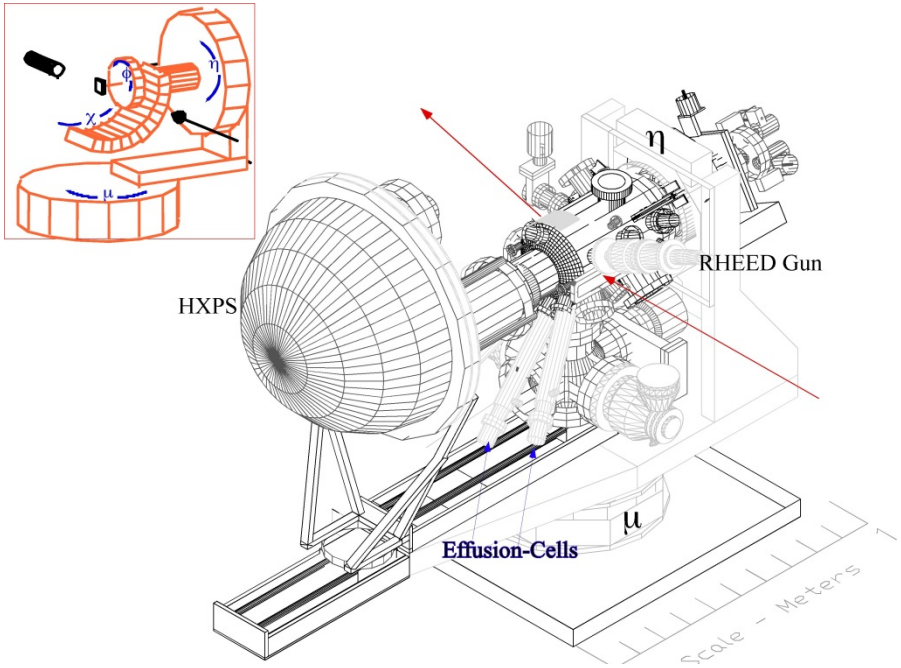
APL 98, 132102 (2011) *S.J.A & S.S.*



PRB 82, 081103 (2010) *S.J.A & S.S.*

Hybrid oxide MBE for XIS

- Combine Metallorganic sources with thermal sources (ALD and MBE).
- Combine fundamental science of correlated electron materials with industrial relevant materials – (see recent report of SiO_2 doped HfO_2 ferroelectric transistor)
- Proposal to NSF with industry contribution include MRSEC PIs.



From Bedzyk et al. proposal to the NSF.