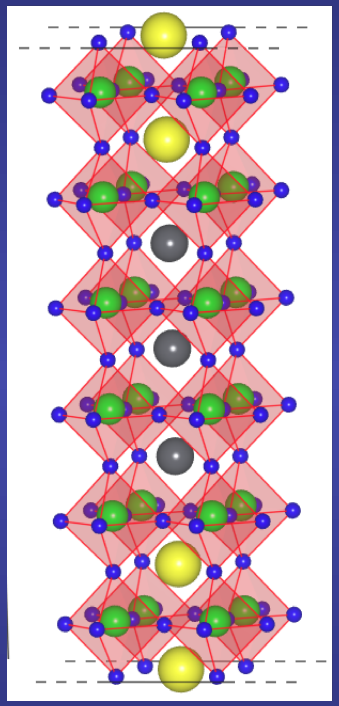
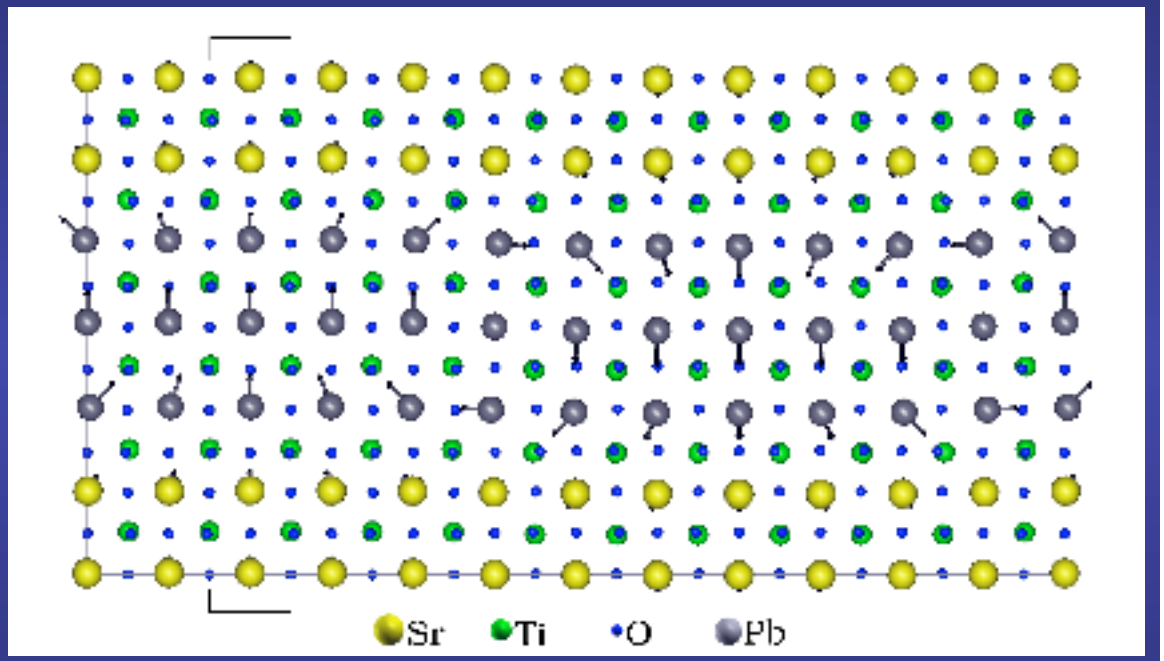
First-principles simulations on $PbTiO_3/SrTiO_3$ superlattices





Javier Junquera

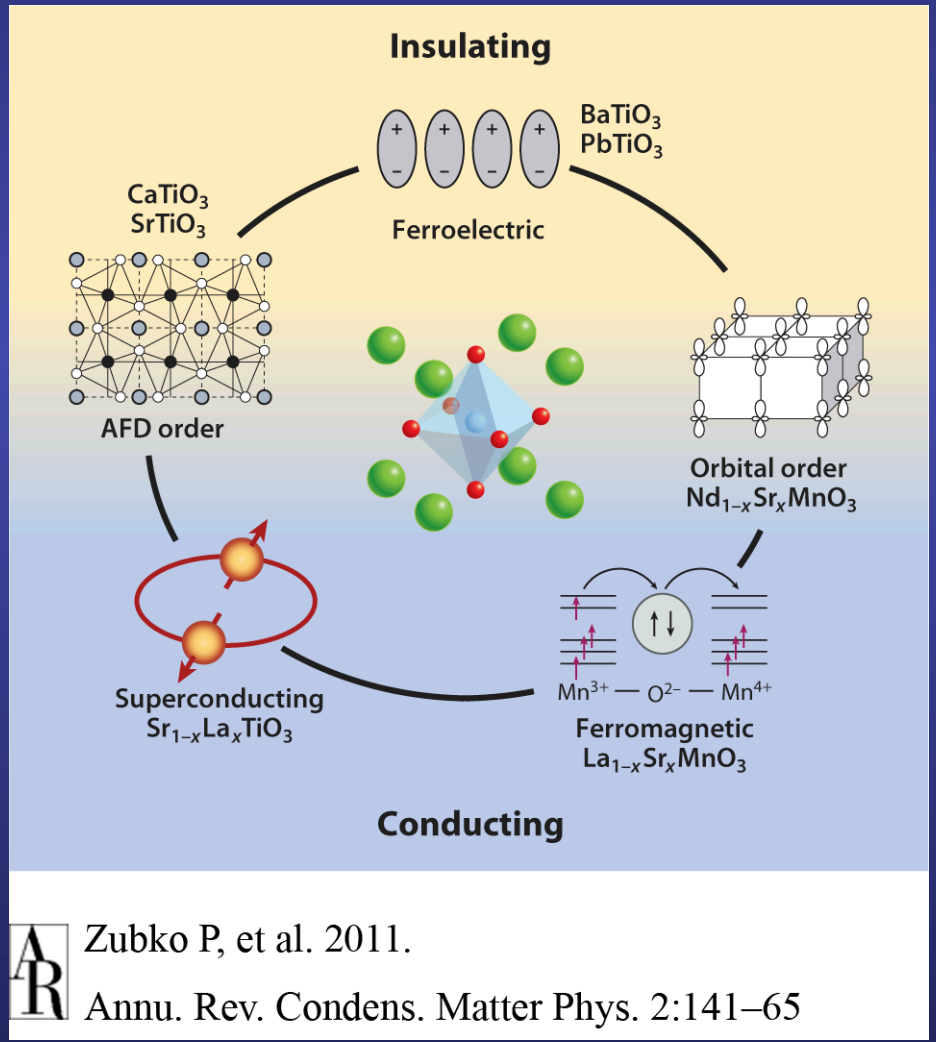
Pablo Aguado-Puente

Pablo García-Fernández

UC
UNIVERSIDAD DE CANTABRIA

Multitude of fascinating and exotic properties boasted by transition metal oxides

ABO_3 perovskites oxides: simple structure, wide variety of properties

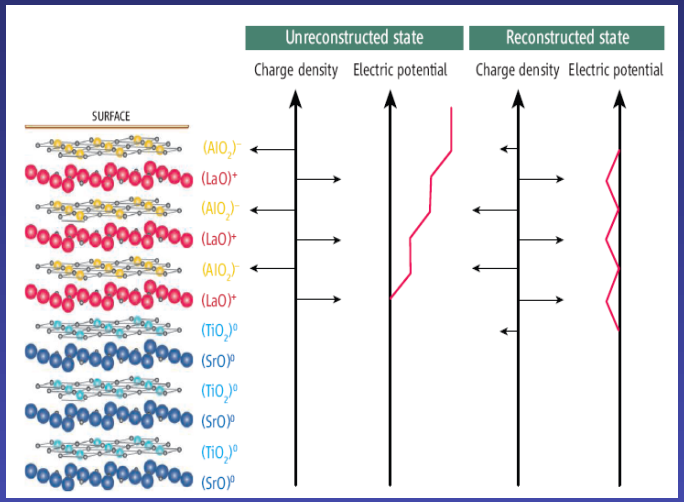


Zubko P, et al. 2011.

Annu. Rev. Condens. Matter Phys. 2:141–65

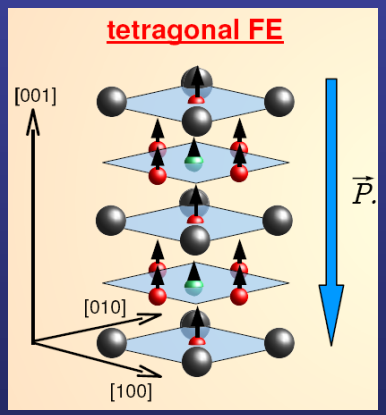
Some surprises at the interfaces between two oxides

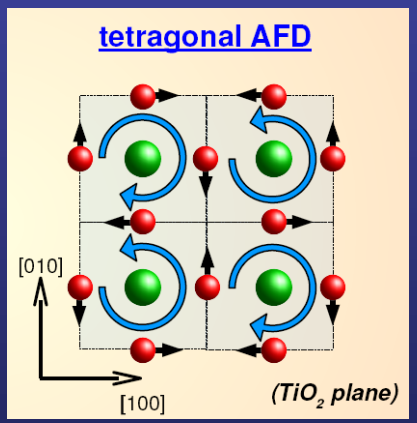
The interface between two good insulators (e.g. $LaAlO_3$ and $SrTiO_3$) is metallic



A. Ohtomo and H. Y. Hwang, Nature 427, 423 (2004)

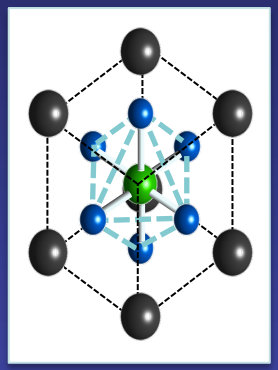
Appearance of improper ferroelectricity in $PbTiO_3/SrTiO_3$ superlattices





E. Bousquet *et al.*, Nature 452, 732 (2008)

Many instabilities might be present in bulk ABO_3 perovskites: They often compete and tend to suppress each other

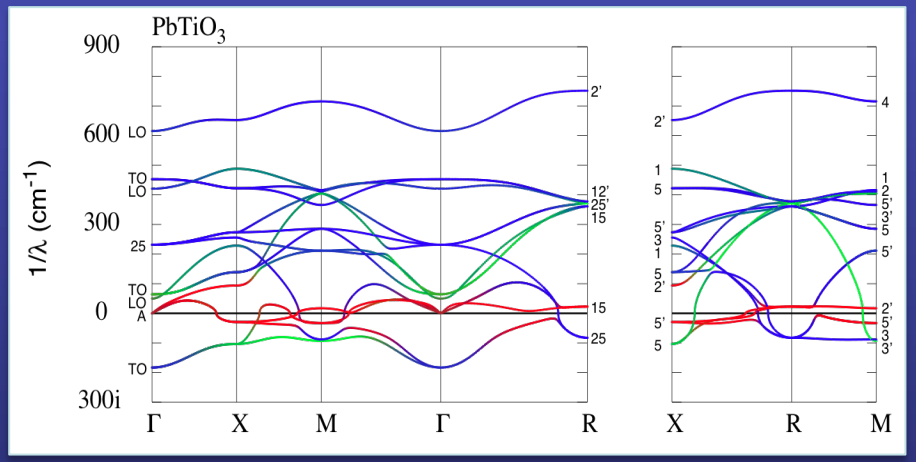


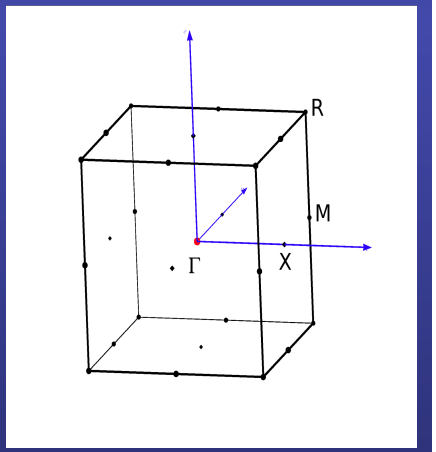
"ideal" cubic perovskite structure,
taken as the high-symmetry reference configuration

Stable only within a narrow range of ionic radii.

Ph. Ghosez *et al.*, Phys. Rev. B 60, 836 (1999)

Phonon dispersion curves at the bulk cubic experimental lattice constant

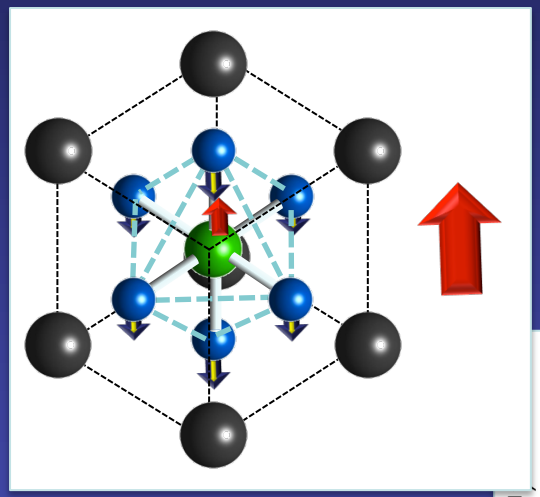




Signature of the instability:
a branch in the phonon dispersion curve with imaginary frequency

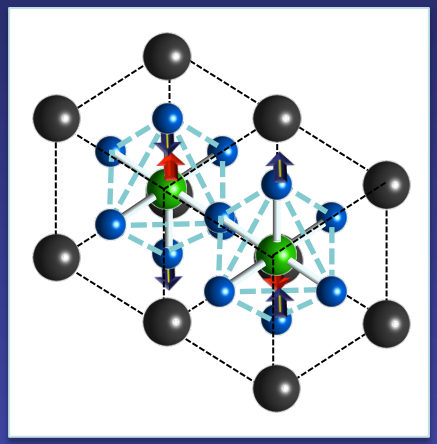
Typical crystal instabilities

Γ-point
(0.0, 0.0, 0.0)



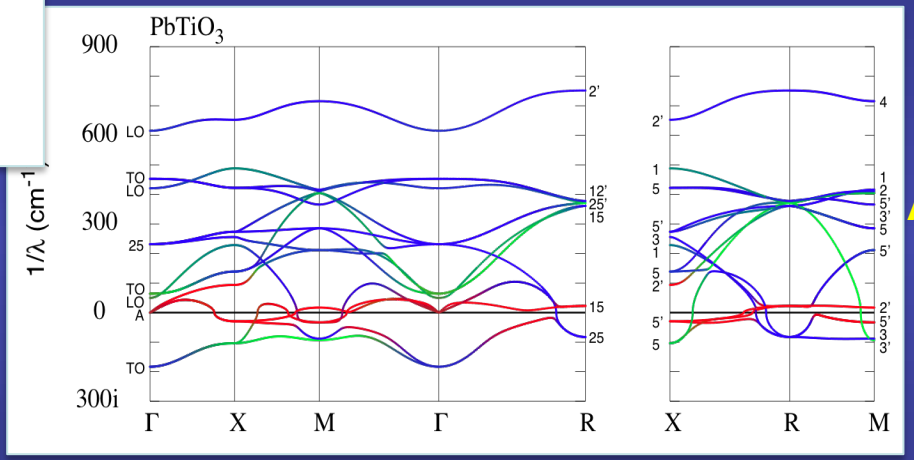
Ferroelectric (FE)

X-point
(0.5, 0.0, 0.0)

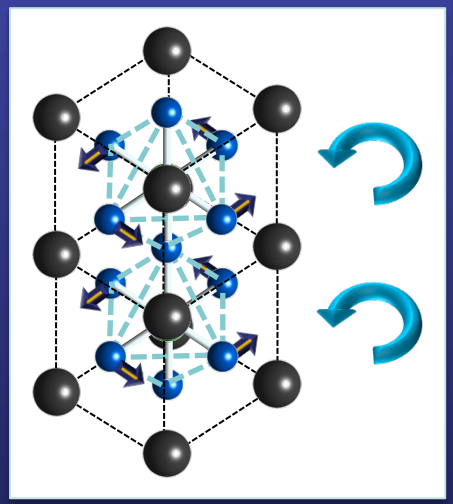


Antiferroelectric (AFE)

Ph. Ghosez *et al.*, Phys. Rev. B 60, 836 (1999)



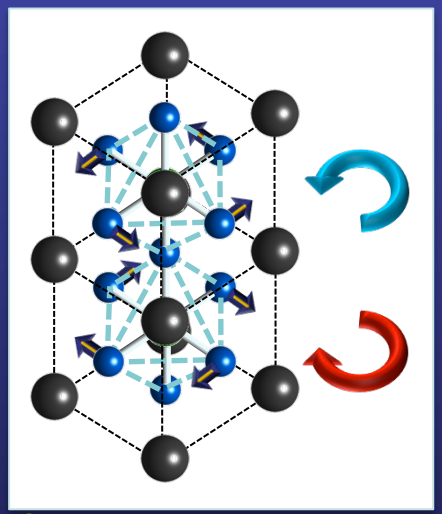
M-point
(0.5, 0.5, 0.0)



Antiferrodistortive (AFD)

PbTiO$_3$ phonon dispersion curves at the bulk cubic experimental lattice constant

R-point
(0.5, 0.5, 0.5)



Antiferrodistortive (AFD)

The competition between all the structural instabilities might be altered at surfaces/interfaces

Surface might induced reconstructions to saturate dangling bonds

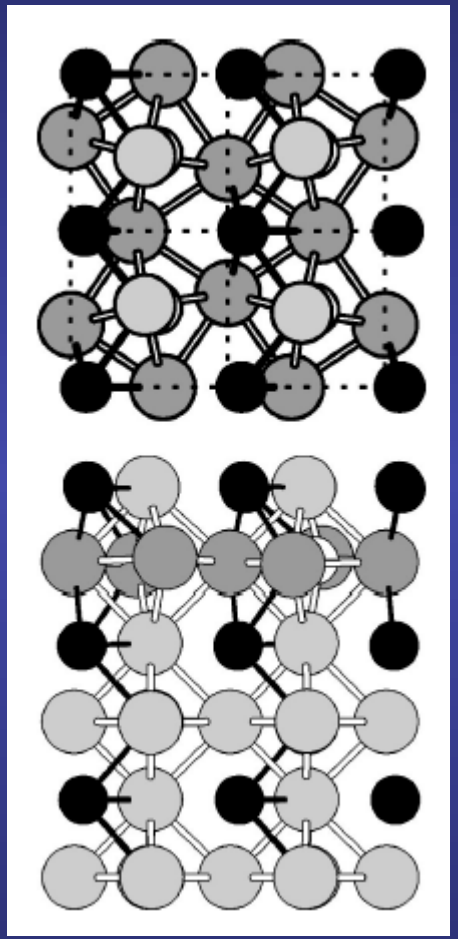
(001) $PbTiO_3$

c(2×2) reconstructions in PbO-terminated

- Substantial enhancement of the AFD distorsion
- Driving force: **shorter PbO bonds**

⇓

- Not observed neither in TiO_2 termination nor $BaTiO_3$ surface



A. Munkholm *et al.*, Phys. Rev. Lett. 88, 016101 (2002)

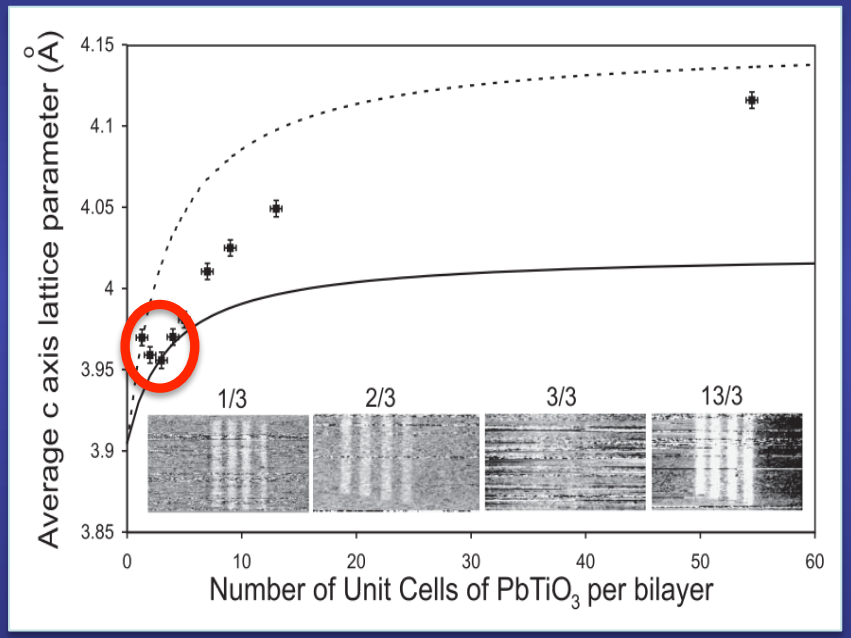
C. Bungaro and K. M. Rabe, Phys. Rev. B 71, 035420 (2005)

$PbTiO_3/SrTiO_3$ superlattice: polarization, c/a, and phase transition T can be monitored with PTO volume

Tetragonality

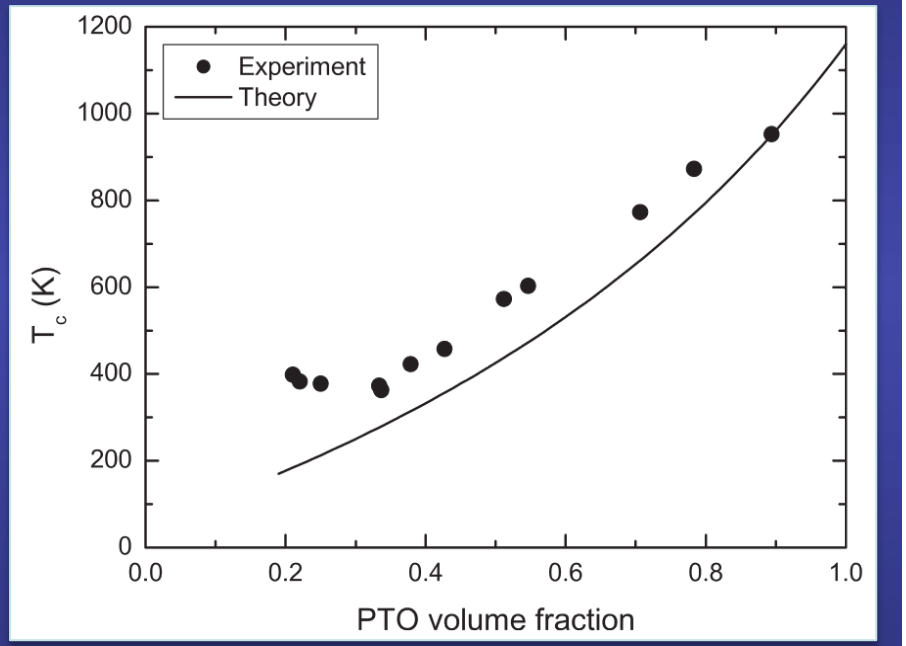
(related with P due to the large polarization-strain coupling in $PbTiO_3$)

M. Dawber *et al.*, Phys. Rev. Lett. 95, 177601 (2005)



Phase transition temperature

M. Dawber *et al.*, Adv. Mater. 19, 4153 (2007)



In the experiment, the number of layers of $SrTiO_3$, n_s, was fixed to 3

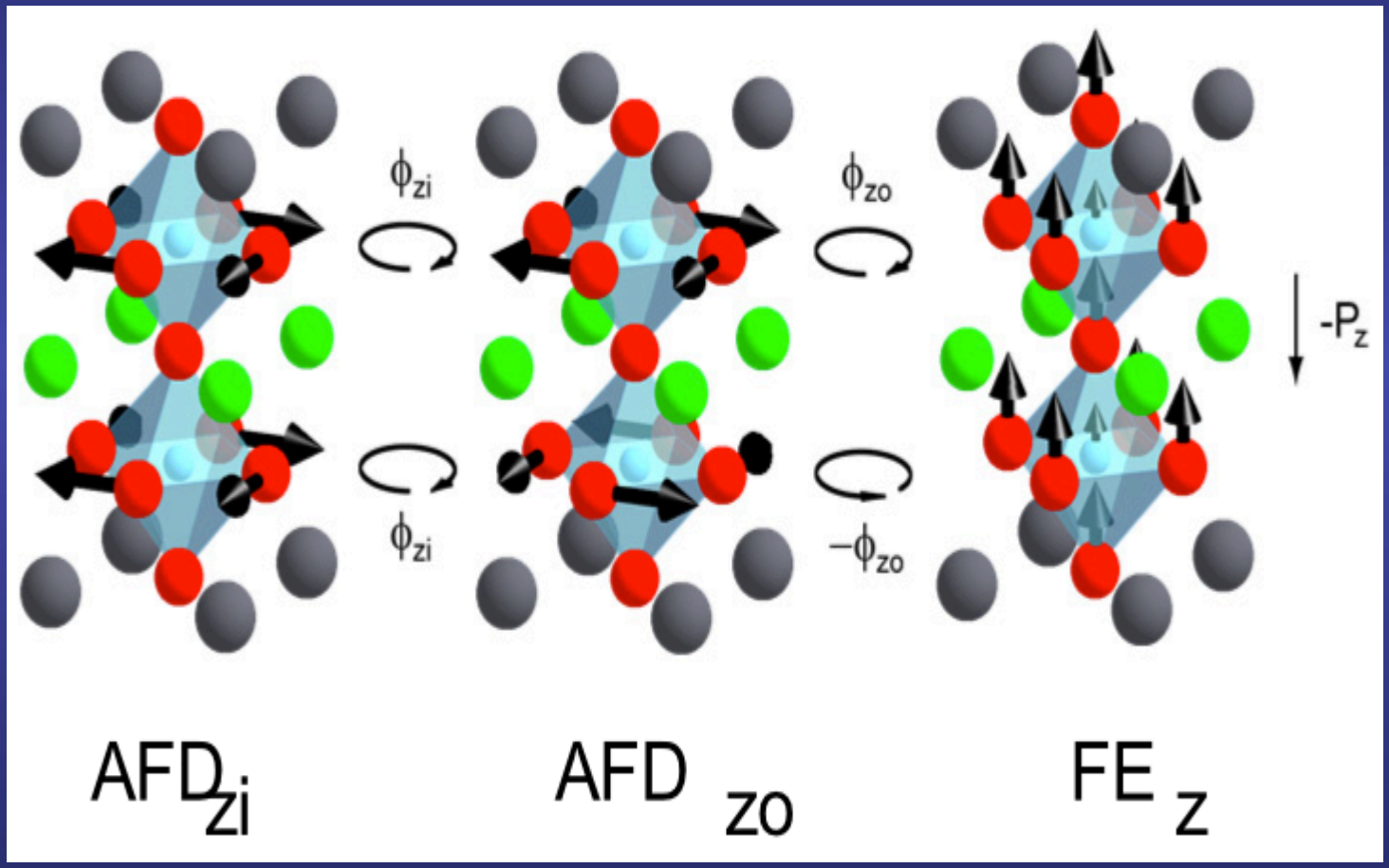
For $PbTiO_3$ layers thickness larger than 3, $n_p/n_s > 1$, the polarization is found to be reduded (depolarizing field effect)

For $PbTiO_3$ layer thickness smaller than 3, $n_p/n_s<1$,unexpected recovery of ferroelectricity that can not be accounted for by simple electrostatic arguments

Short-period $PbTiO_3/SrTiO_3$ superlattices: the GS involves trilinear coupling between two AFD modes and a polar FE mode

Improper ferroelectricity

E. Bousquet *et al.*, Nature 452, 732 (2008)



In-phase AFD rotations of O octahedra

Out-of-phase AFD rotations of O octahedra

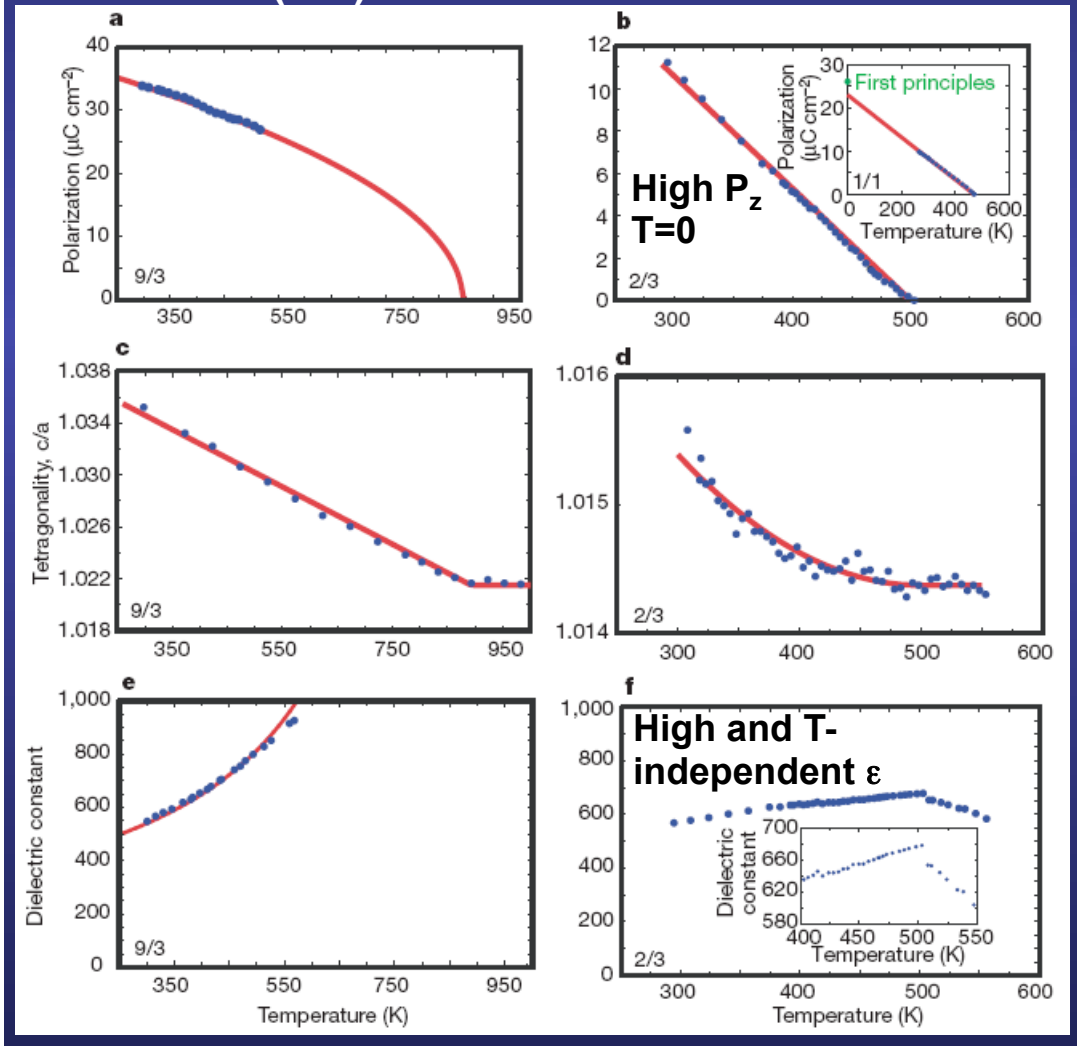
Ferroelectric mode

Interesting and useful features of improper ferroelectrics

E. Bousquet *et al.*, Nature 452, 732 (2008)

N. Sai *et al.*, Phys. Rev. Lett. 102, 107601 (2010)

Normal sample (9/3) | **Anomalous sample (2/3)**



Reduced sensitive to depolarizing fields

The instability to a single domain ferroelectric state does not vanish even when depolarizing field remains unscreened

P_s ($YMnO_3$ thin films) ≈ P_s($YMnO_3$ bulk)

N. A. Benedek and C. J. Fennie, Phys. Rev. Lett. 106, 107204 (2011)

Promising way of generating novel magnetoelectric couplings

Possible paths for electric-field switching of magnetization in $Ca_3Mn_2O_7$

First-principles study on $PbTiO_3/SrTiO_3$ superlattices

Influence of the epitaxial strain

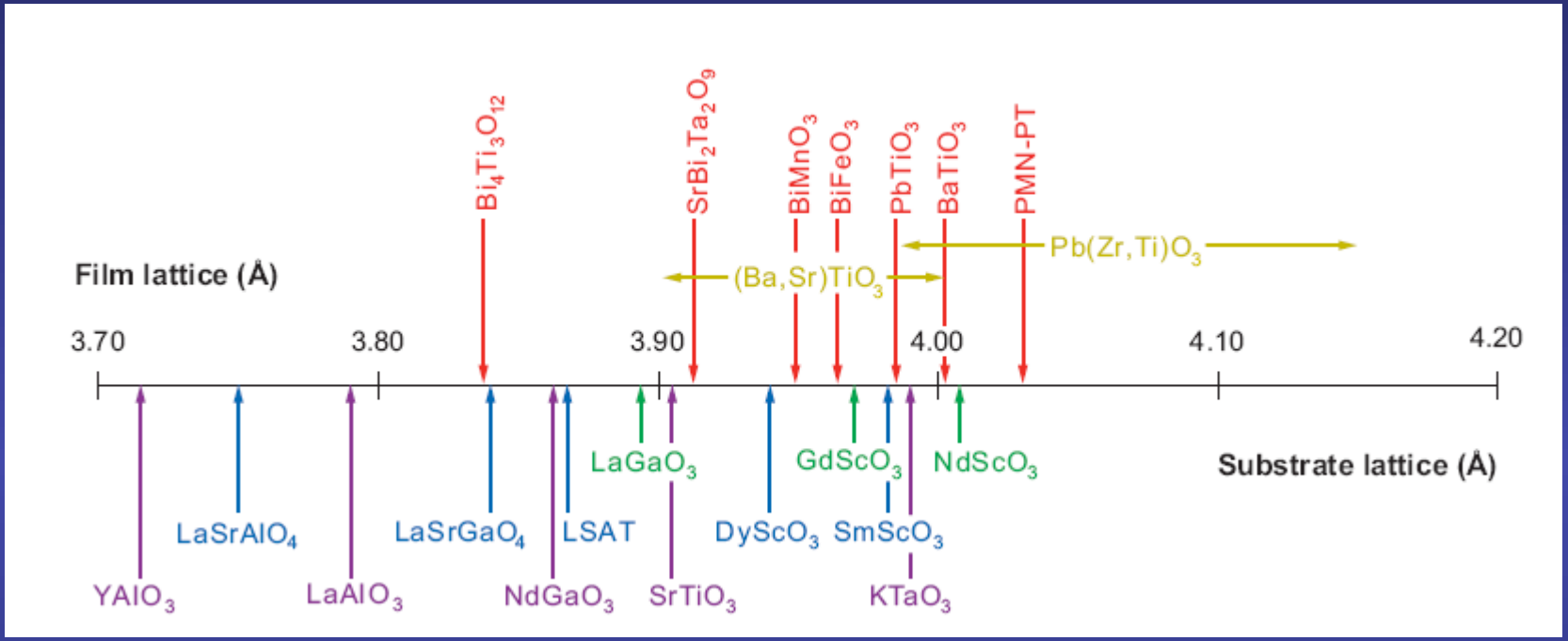
Eventual stabilization of domains

First-principles study on $PbTiO_3/SrTiO_3$ superlattices

Influence of the epitaxial strain

Eventual stabilization of domains

Current interest in functional oxides is largely based on engineered epitaxial thin films



D. G. Schlom *et al.*, Annu. Rev. Mater. Res. 37, 589 (2007)

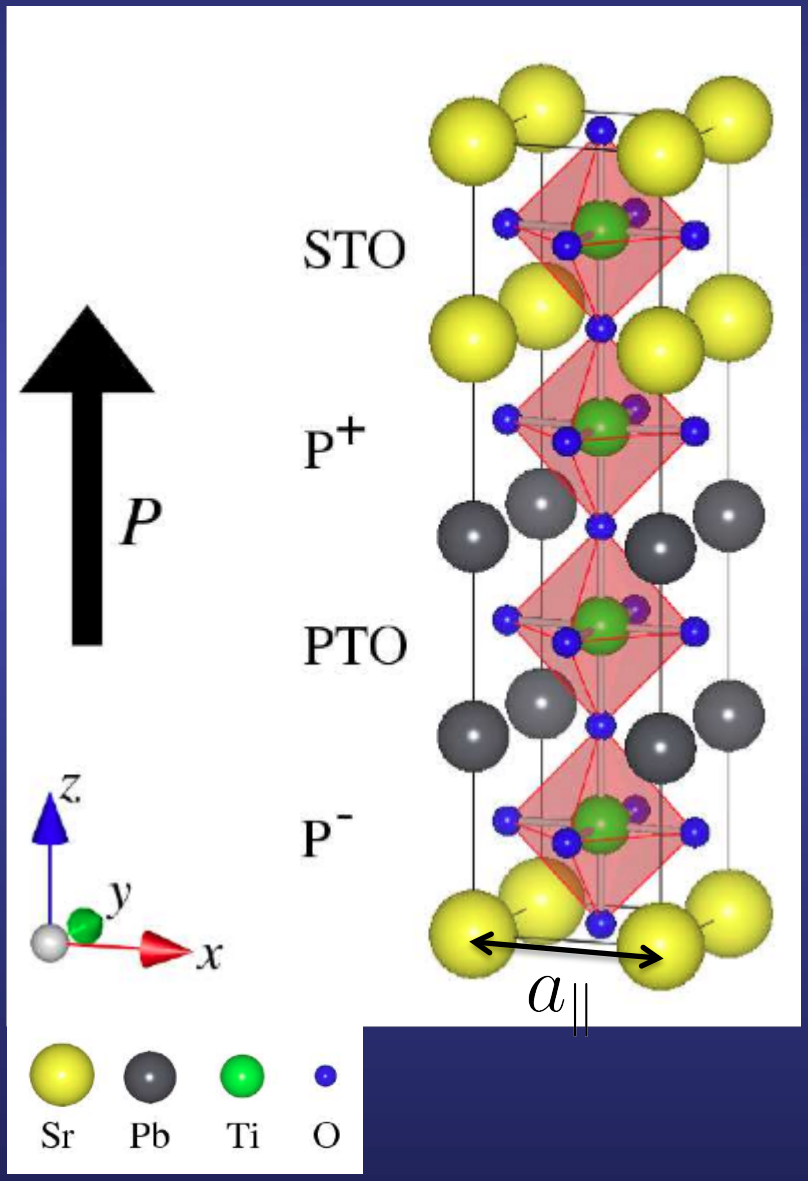
Many oxides have similar lattice constants allowing for a good match at the interfaces

What would happen if we could mix materials with different properties?

Potential for novel behaviour

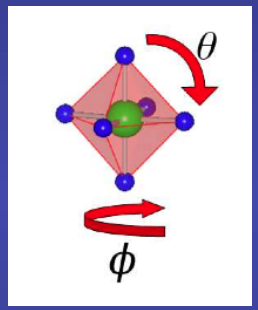
First-principles simulations on monodomain $PbTiO_3/SrTiO_3$ superlattices

(2/2) superlattice



Local Density Approximation (LDA)

(2 × 2) in-plane periodicity to allow for TiO_6 octahedra rotations ϕ and tiltings θ



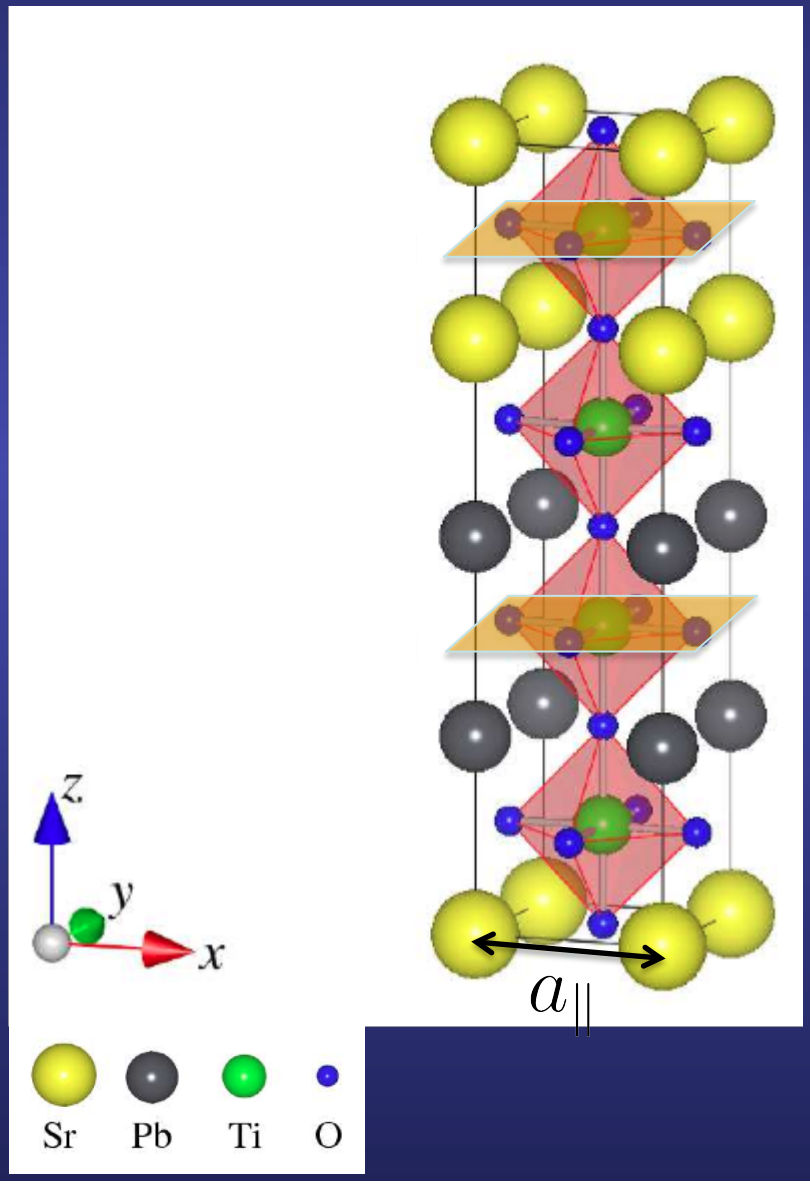
Mechanical boundary conditions implicitly treated by fixing the in-plane lattice constant

Short-circuit electrical boundary conditio

Oxygen octahedra labeled according to:
- chemical identity of first two neighbours layers
- polarization

First-principles atomic relaxations on monodomain $PbTiO_3/SrTiO_3$ superlattices

(2/2) superlattice

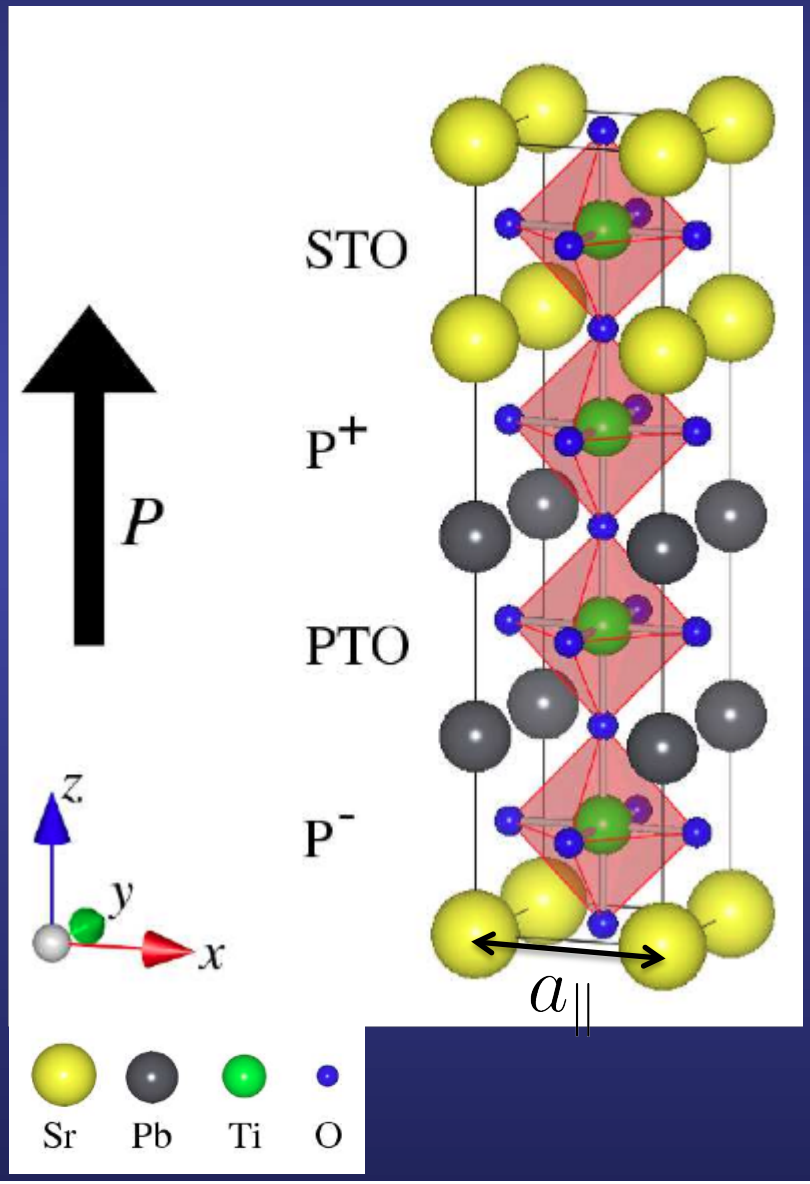


Step 1:
Getting a reference non-polar structure

Relaxation of the atomic position and lattice vectors
BUT
With some constraints to avoid the appearance of a polarization

First-principles atomic relaxations on monodomain $PbTiO_3/SrTiO_3$ superlattices

(2/2) superlattice

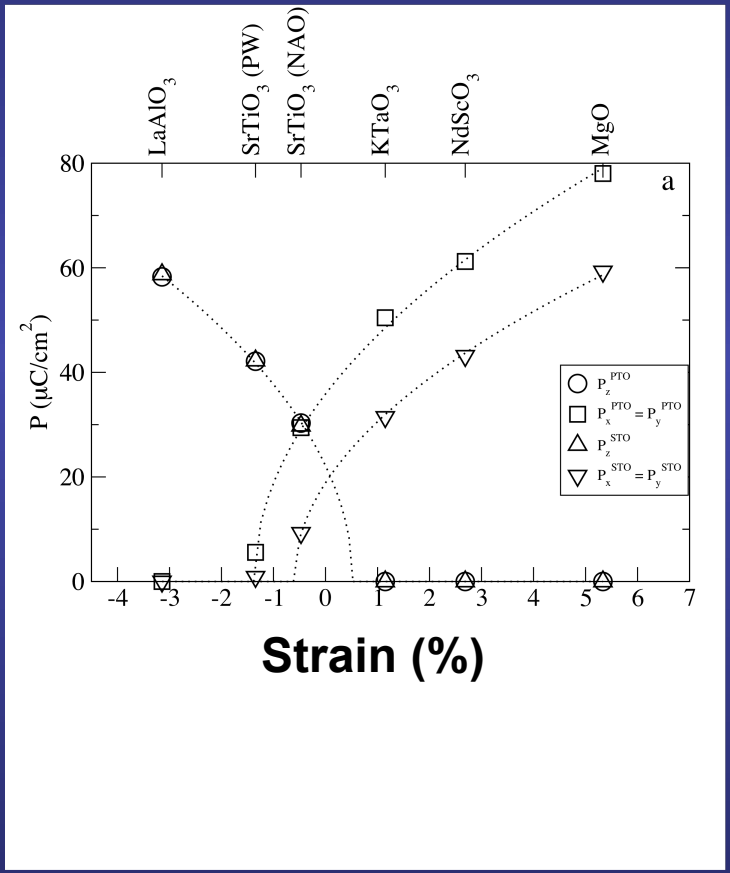


Step 2:
Getting the most stable phases

Starting from the most stable non-polar phase,
SYMMETRY IS BROKEN
A new atomic relaxation is performed

Polarization-strain coupling in monodomain $PbTiO_3/SrTiO_3$ (2/2) superlattices

Common cubic substrates



PW: $SrTiO_3$ lattice constant using plane wave 3.84 Å

NAO: $SrTiO_3$ lattice constant using numerical atomic orbitals (3.87 Å)

For **compressive strains**:

-homogeneous polarization stabilized along z (*c*-phase)

-P_z preserved at the $PbTiO_3/SrTiO_3$ interface (electrostatic restriction)

For **tensile strains**:

-polarization lies along [110] direction (*aa*-phase)

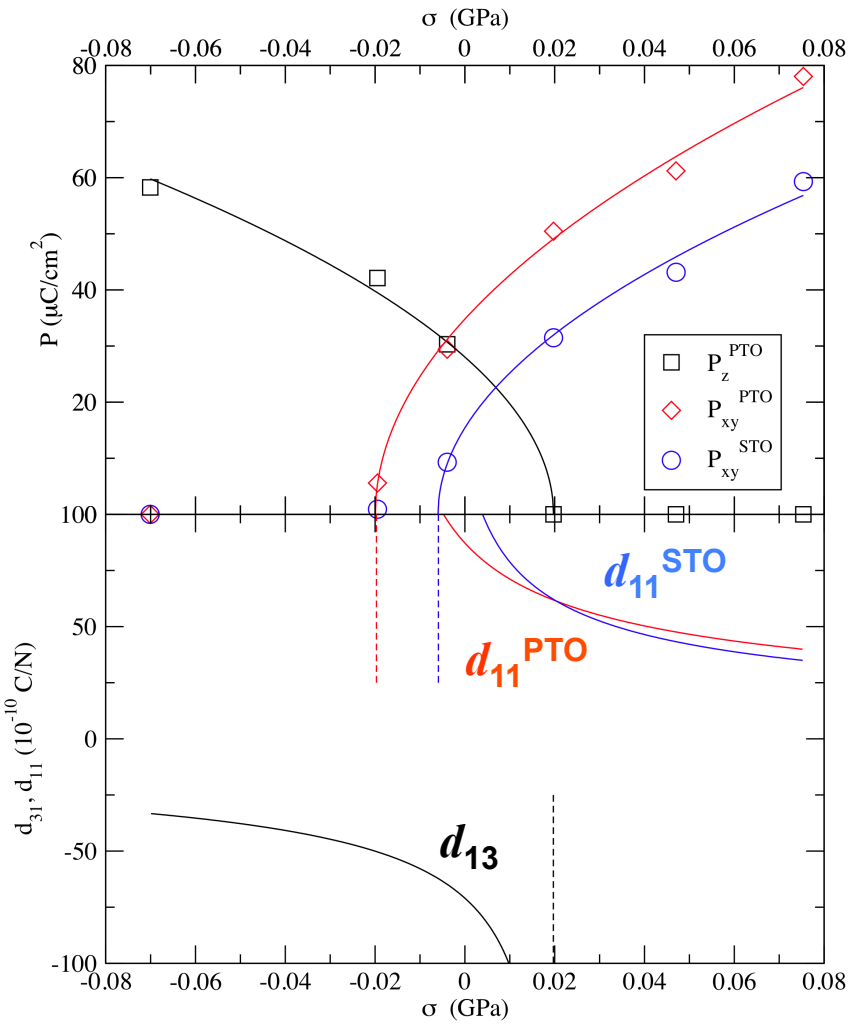
-no electrostatic restriction to keep the in-plane polarization at the same value

For **intermediate regime:**

-continuous rotation of polarization (*r*-phase)

-second order phase transitions

Large electromechanical response in monodomain $PbTiO_3/SrTiO_3$ (2/2) superlattices

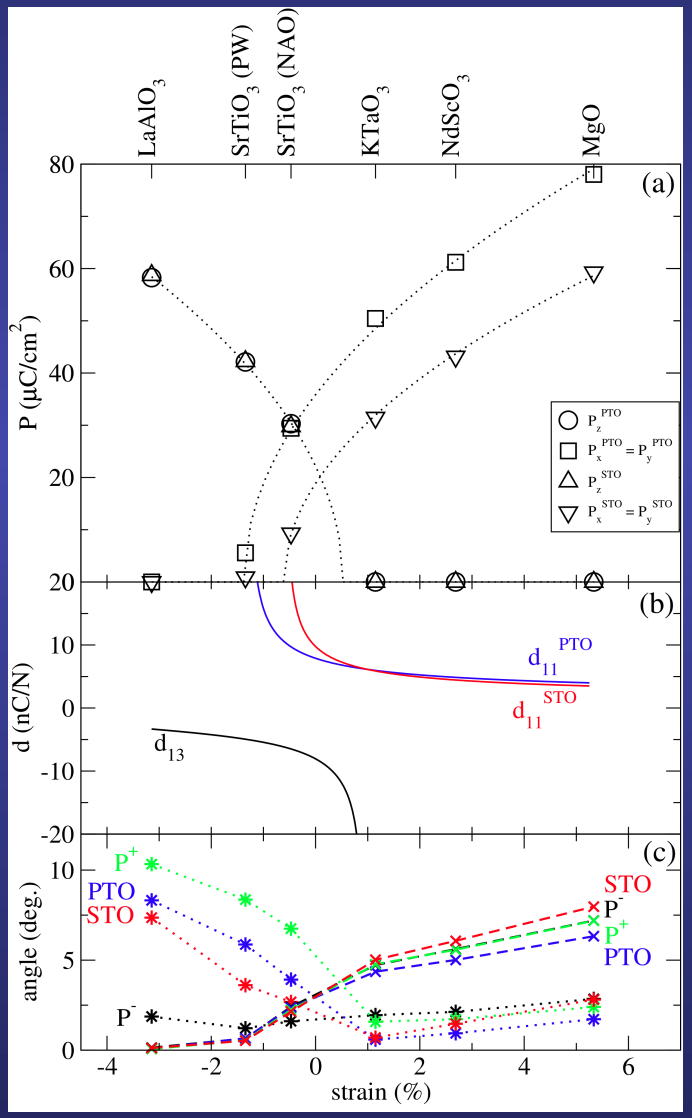


Polarization as a function of stress

Piezoelectric components diverge in a region very accesible experimentally, around lattice constant of $SrTiO_3$

FE-AFD-strain coupling in monodomain $PbTiO_3/SrTiO_3$ (2/2) superlattices

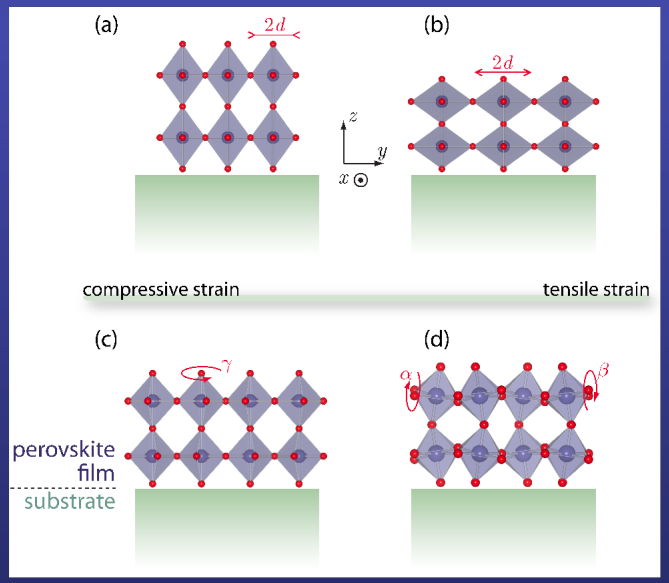
Common cubic substrates



* : rotations

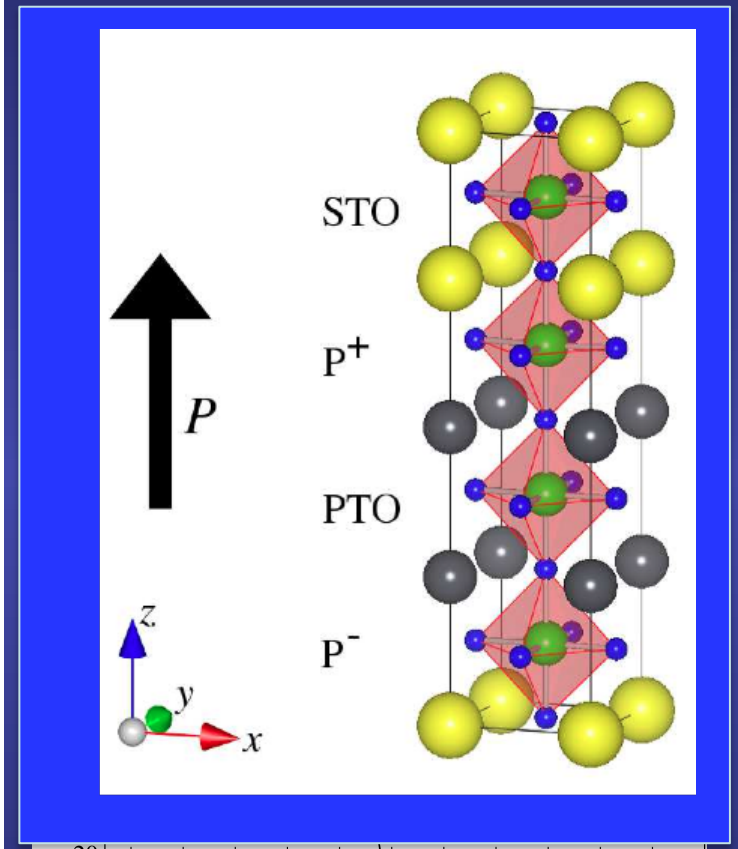
Compressive strains favour rotation of the TiO_6 octahedra

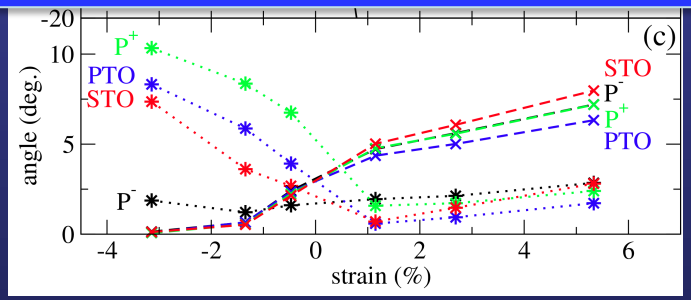
Tensile strains favour tilting of the TiO_6 octahedra



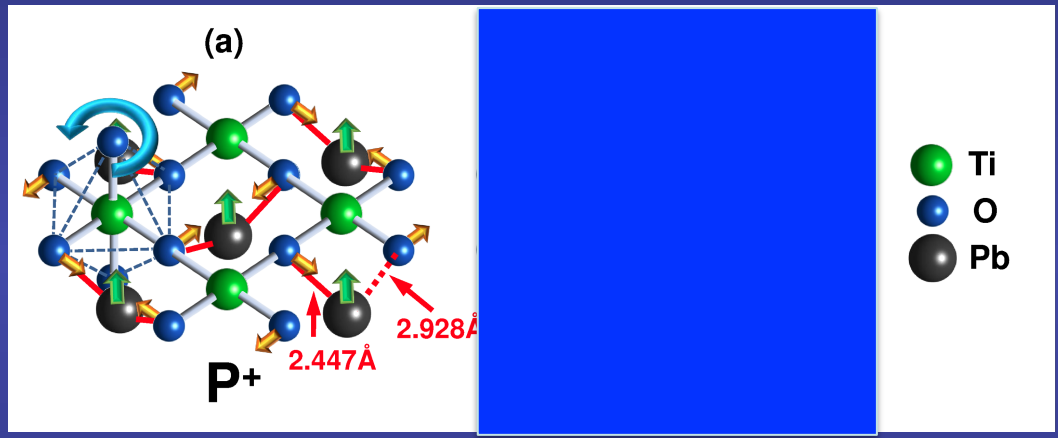
J. Rondinelli and N. A. Spaldin, cond-mat/1103.4418

Behaviour of the different TiO_6 octahedra explained by a covalent model





When a large compressive strains are applied, P^+ rotates more than P^-.

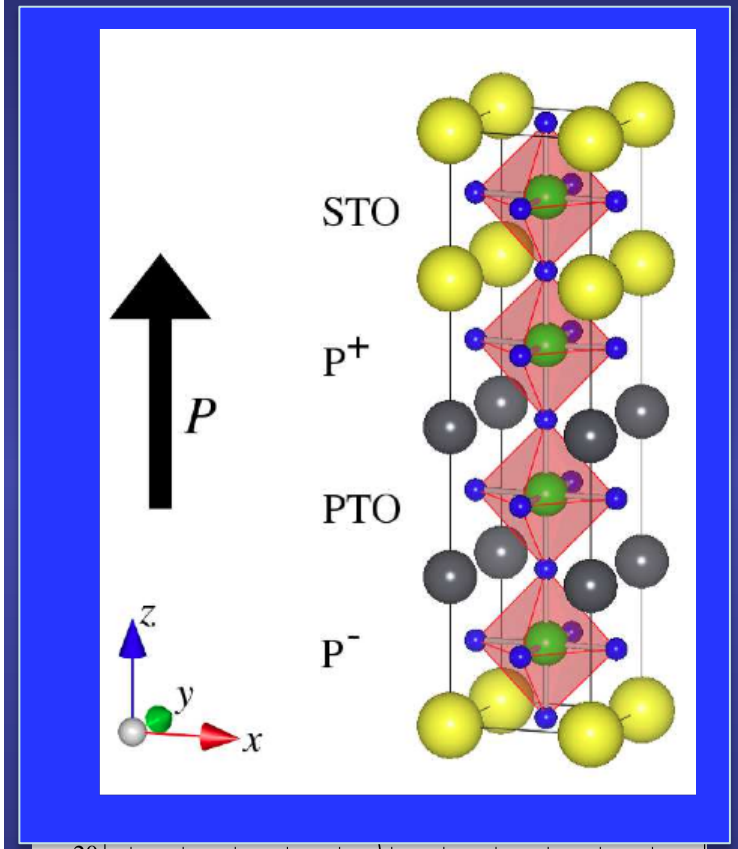


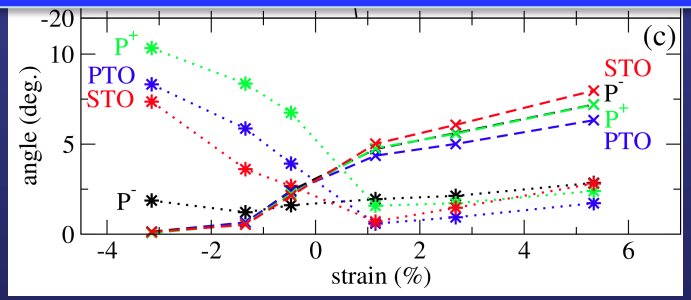
TiO_2 layer and Pb atoms below

When Pb atom moves up (FE), O moves towards it to form stronger covalent bonds

Reinforcement of the P^+ TiO_6 rotation

Behaviour of the different TiO_6 octahedra explained by a covalent model

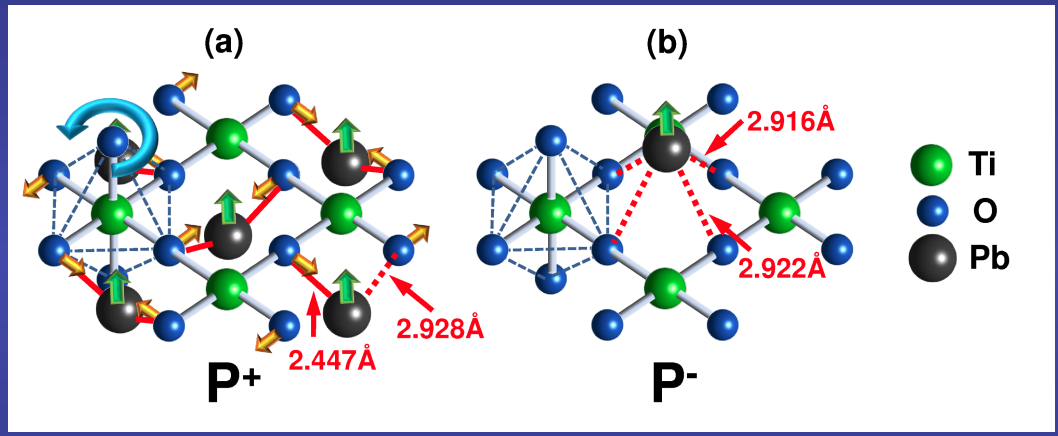




* : rotations

x :

When a large compressive strains are applied, P^+ rotates more than P^-.



TiO_2 layer and Pb atoms below	TiO_2 layer and Pb atom up
When Pb atom moves up (FE), O moves towards it to form stronger covalent bonds	When Pb atom moves up (FE) all Pb-O bonds are weakened
Reinforcement of the P^+ TiO_6 rotation	Reduction of the P^- TiO_6 rotation

Monodomain $PbTiO_3/SrTiO_3$ superlattices with different periodicities

In-plane lattice constant: theoretical $SrTiO_3$ (3.874 Å)

	(1/1)			(2/2)			(3/3)		
	P_{STO}	P_{PTO}	E	P_{STO}	P_{PTO}	E	P_{STO}	P_{PTO}	E
Para.	(0.0, 0.0, 0.0)	(0.0, 0.0, 0.0)	+30.6	(0.0, 0.0, 0.0)	(0.0, 0.0, 0.0)	+51.3	(0.0, 0.0, 0.0)	(0.0, 0.0, 0.0)	+58.4
[110]	(20.7, 20.7, 0.0)	(31.4, 31.4, 0.0)	+9.2	(16.0, 16.0, 0.0)	(34.5, 34.5, 0.0)	+14.1	(14.2, 14.2, 0.0)	(35.9, 35.9, 0.0)	+20.7
[001]	(0.0, 0.0, 35.5)	(0.0, 0.0, 35.0)	+2.3	(0.0, 0.0, 34.4)	(0.0, 0.0, 34.8)	+12.5	(0.0, 0.0, 33.6)	(0.0, 0.0, 34.3)	+24.2
[111]	(14.2, 14.2, 31.5)	(23.3, 23.3, 31.1)	GS	(9.2, 9.2, 29.8)	(29.5, 29.5, 30.4)	GS	(6.9, 6.9, 29.0)	(31.8, 31.8, 30.3)	GS

Independently of the periodicity: the ground state

- always in-plane and out-of-plane polarization

(although for n=1, essentially degenerated with the [001] configuration found in E. Bousquet *et al*. 452, 732 Nature (2008)

- n ≥ 2, pointing along the diagonal of the perovskite unit cell in $PbTiO_3$

Reason for the stabilization of the [111] phase:
$PbTiO_3$ likes rotate more than a monotomic decrease of P_z

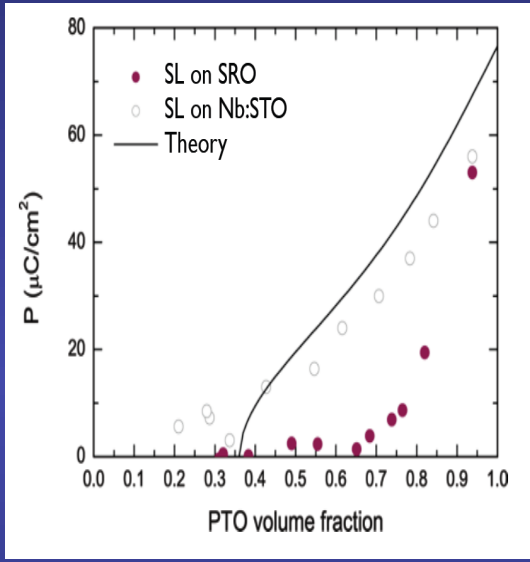
First-principles study on $PbTiO_3/SrTiO_3$ superlattices

Influence of the epitaxial strain

Eventual stabilization of domains

Structural and dielectric properties of PTO/STO superlattices as a function of the periodicity, electrodes and electric fields

Remnant polarization as a function of the $PbTiO_3$ volume fraction



Nb-doped $SrTiO_3$/…/$PbTiO_3$/$SrTiO_3$/…/Au

Follows DGL theory (assumes mono)

$SrRuO_3$/…/$PbTiO_3$/$SrTiO_3$/…/$SrRuO_3$

Does not follow DGL theory
Almost 0 remnant polarization except for the highest $PbTiO_3$ volume fractions

Structural parameters almost identical for the two series

Suggest of a polydomain phase with domain wall motion

P. Zubko *et al.*, Phys. Rev. Lett. 104, 187601 (2010)

Tune properties by changing periodicity, electrodes, …

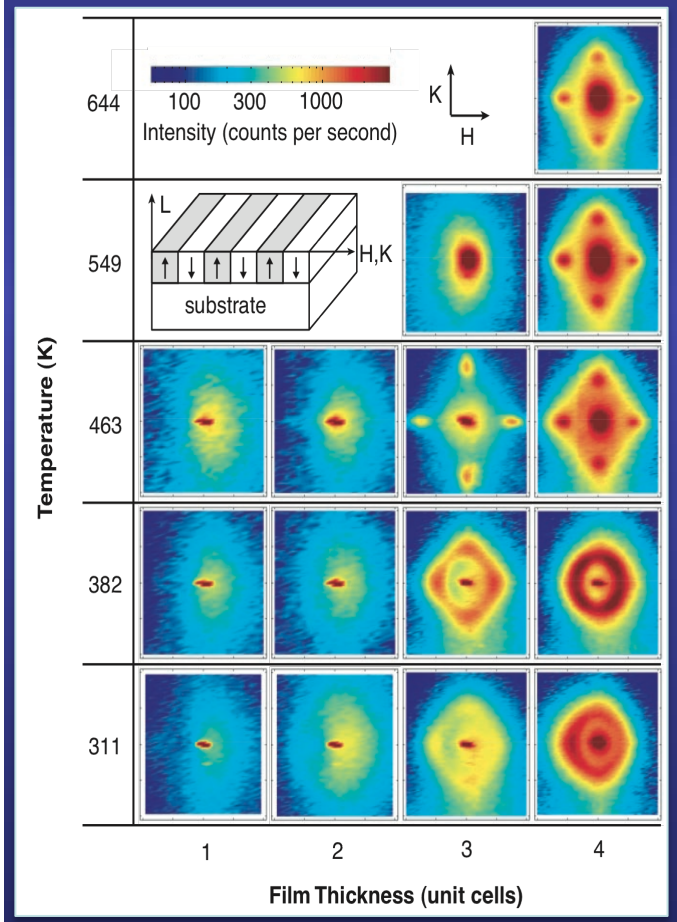
Close competition between mono and polydomain ground state

Ideal system for the study of nanodomains under applied electric fields using x-ray diffraction

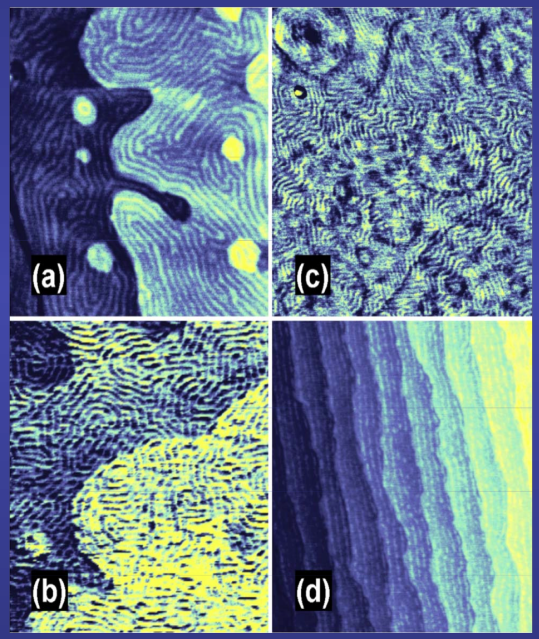
Motivation: study of domains in $PbTiO_3$/$SrTiO_3$ superlattices from first-principles

180° domain structures detected and characterized in $PbTiO_3$ thin films grown on $SrTiO_3$(001) substrates

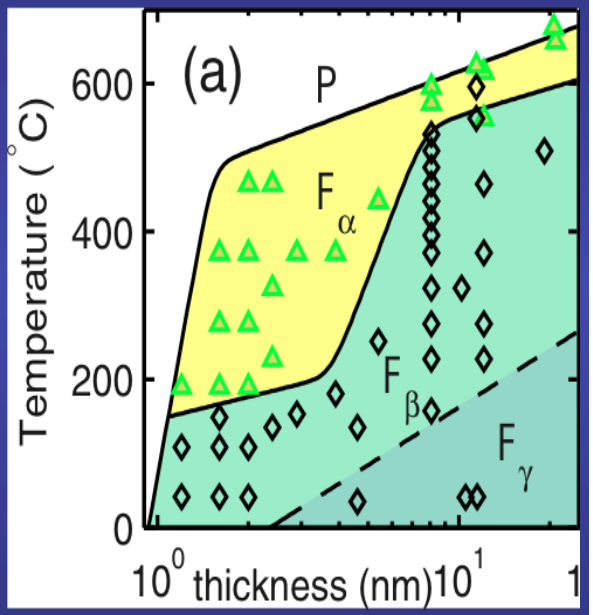
Satellites around $PbTiO_3$ Bragg peaks in synchrotron x-ray



Real space AFM image



Phase diagram



F_α, F_β : domain phases with different periodicities
F_γ : monodomain phase
P : paraelectric

D. D. Fong *et al.*, Science 304, 1650 (2004)

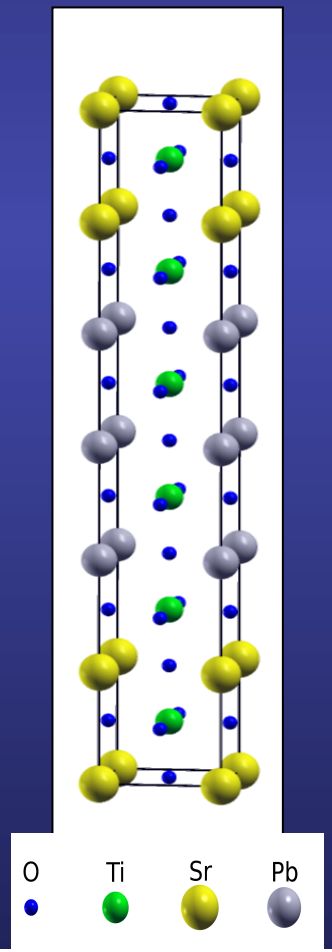
C. Thompson *et al.*, Appl. Phys. Lett. 93, 182901 (2008)

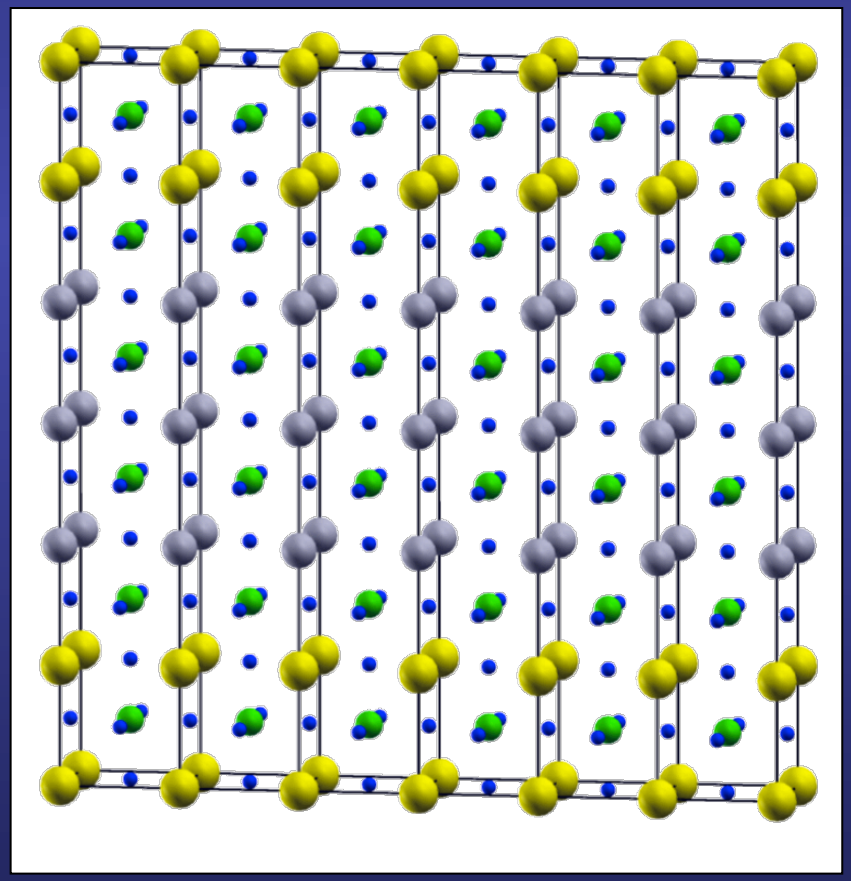
Simulation of domains in $PbTiO_3/SrTiO_3$ superlattices building of the supercell

(3,3) superlattice → 30 atoms

N_x x N_y supercell → Impose lateral size of domains

N_y allows to switch on (N_y =2) and off (N_y = 1) Oxygen octahedra rotations





Example: 6x1 supercell

Simulation of domains in $PbTiO_3/SrTiO_3$ superlattices building of the supercell

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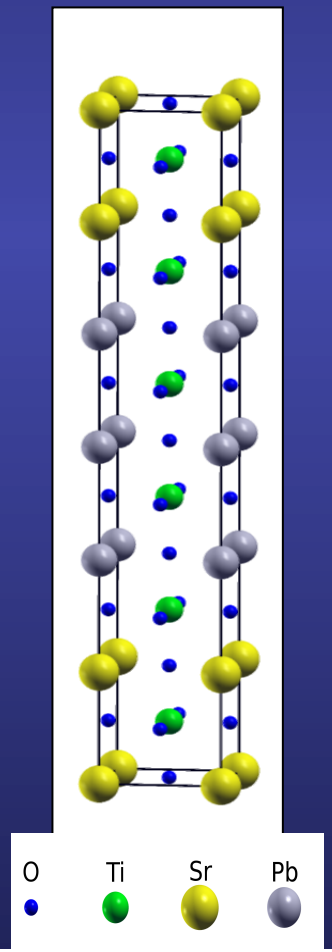
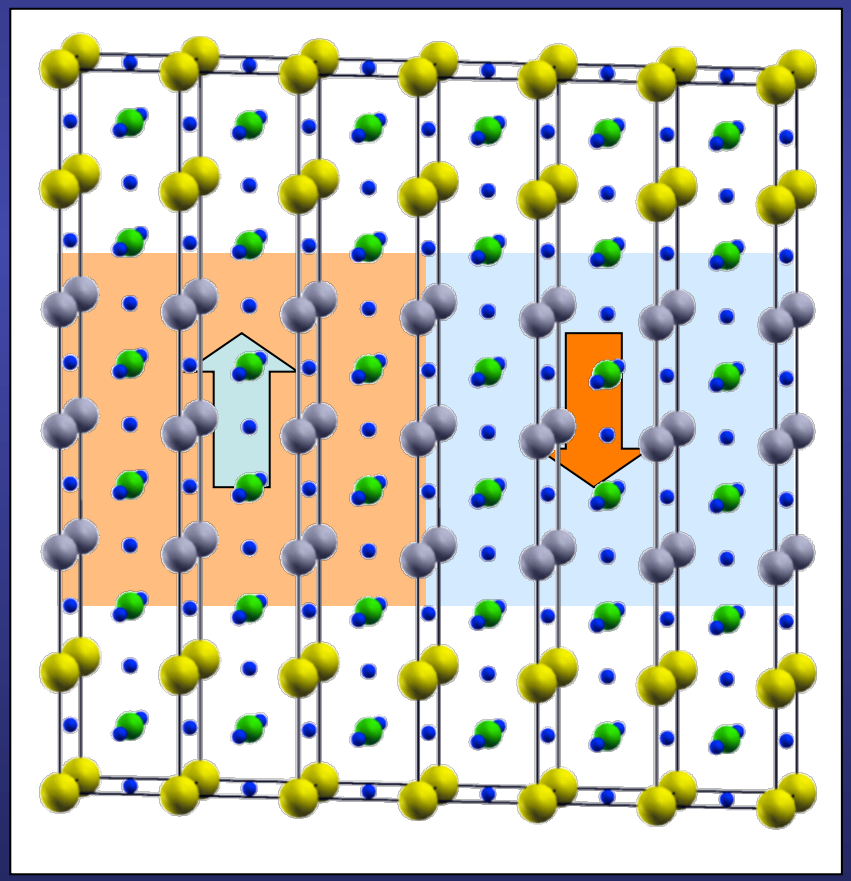
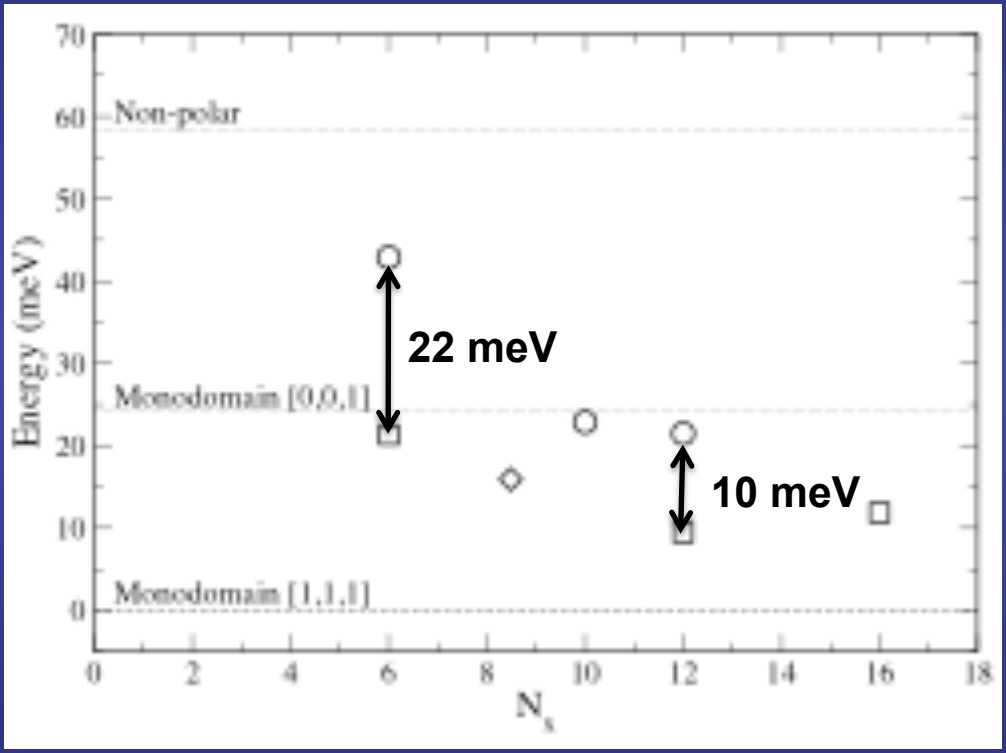




Example: 6x1 supercell

Domains in $PbTiO_3/SrTiO_3$ (3/3) superlattices: Energetics

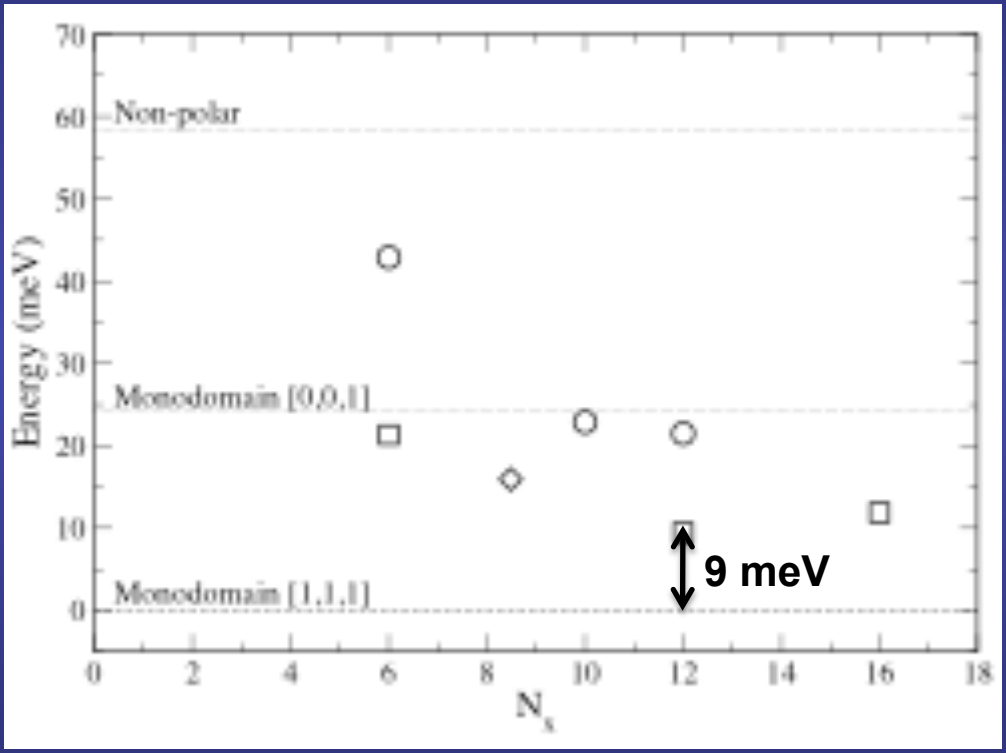


The energy of the polydomain structure decreases with the increase of the domain periodicity (minimum found around N_x =12)

For a given domain periodicity, the energy is lowered if the AFD distortions are allowed (Importance of FE-AFD coupling)

- AFD not allowed
- AFD allowed
- Domain walls along [110]

Domains in $PbTiO_3/SrTiO_3$ (3/3) superlattices: Energetics



○ AFD not allowed
□ AFD allowed
◇ Domain walls along [110]

The energy of the polydomain structure decreases with the increase of the domain periodicity (minimum found around N_x =12)

For a given domain periodicity, the energy is lowered if the AFD distortions are allowed
(Importance of FE-AFD coupling)

The effect of the domain wall orientation is small

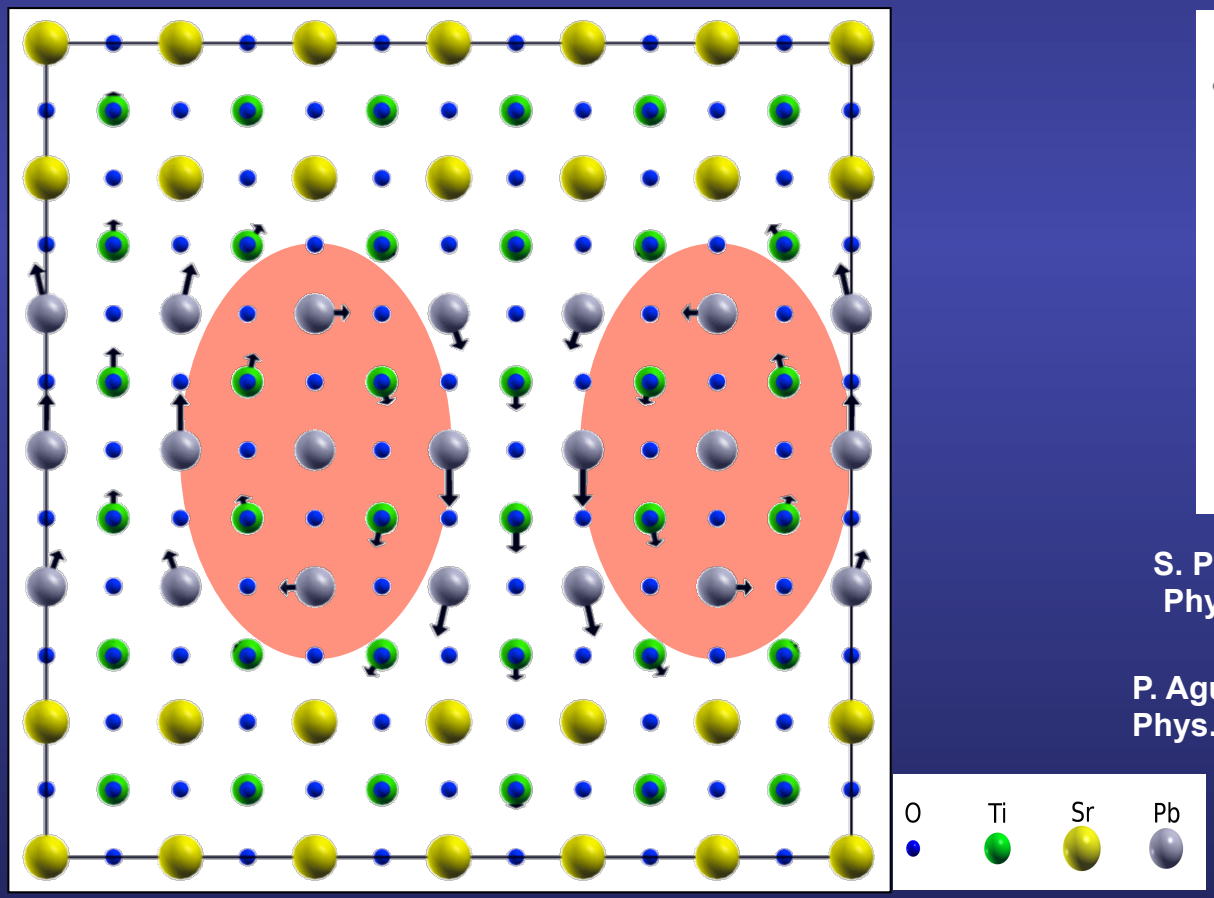
The most stable phase: monodomain
BUT
Difference in energy with respect the most stable polydomain phase small.
Both phases might compete.

Domains in $PbTiO_3/SrTiO_3$ superlattices: adopt the clossure-domain structure with vortices

(3,3) superlattice

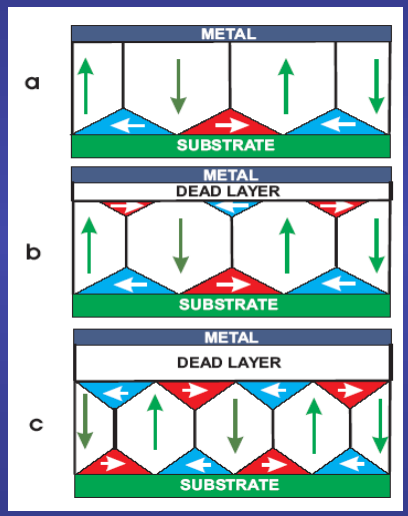
6 unit cells of domain periodicity

Fully relaxed



Vortices at DW

Closed by a large in-plane displacement of the Pb atoms



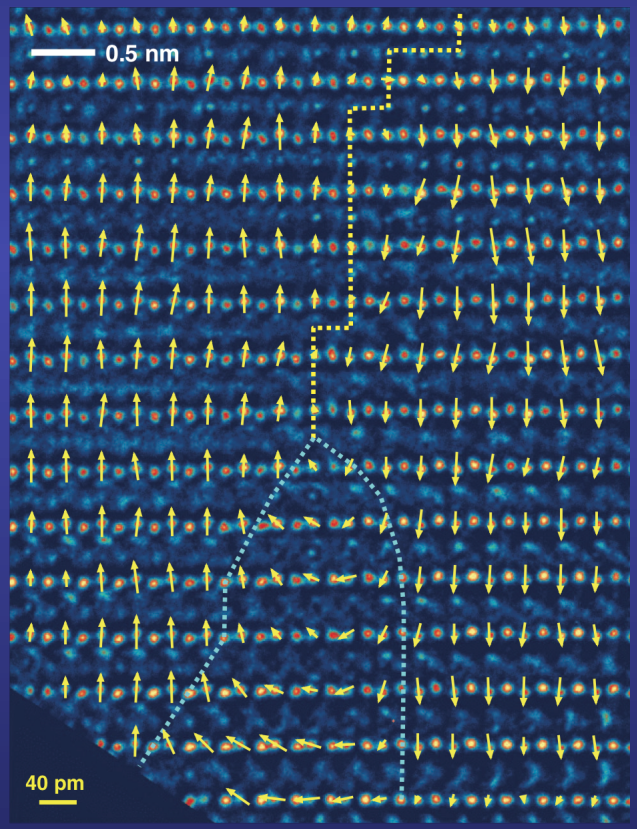
S. Prosandeev and L. Bellaiche, Phys. Rev. B 75, 172109 (2007)

P. Aguado-Puente and J. Junquera Phys. Rev. Lett. 100, 177601 (2008)

Experimental observarion of domains of closure

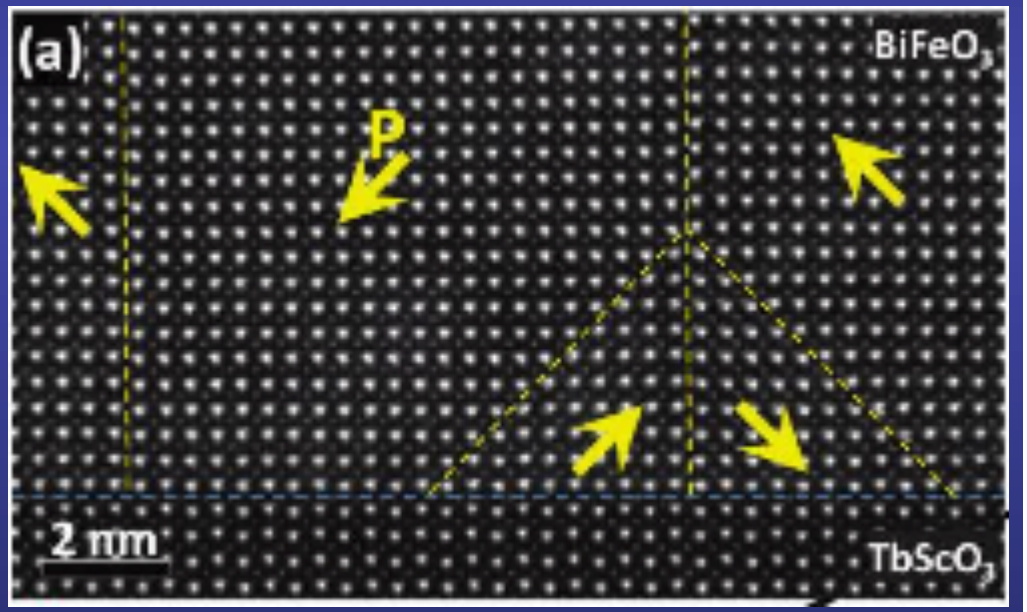
$Pb(Zr_{0.2}Ti_{0.8})O_3/SrTiO_3$

C.-L. Jia *et al.* Science 331, 1420 (2011)



$BiFeO_3/TbScO_3$

C. T. Nelson *et al.* Nano Lett. 11, 828 (2011)



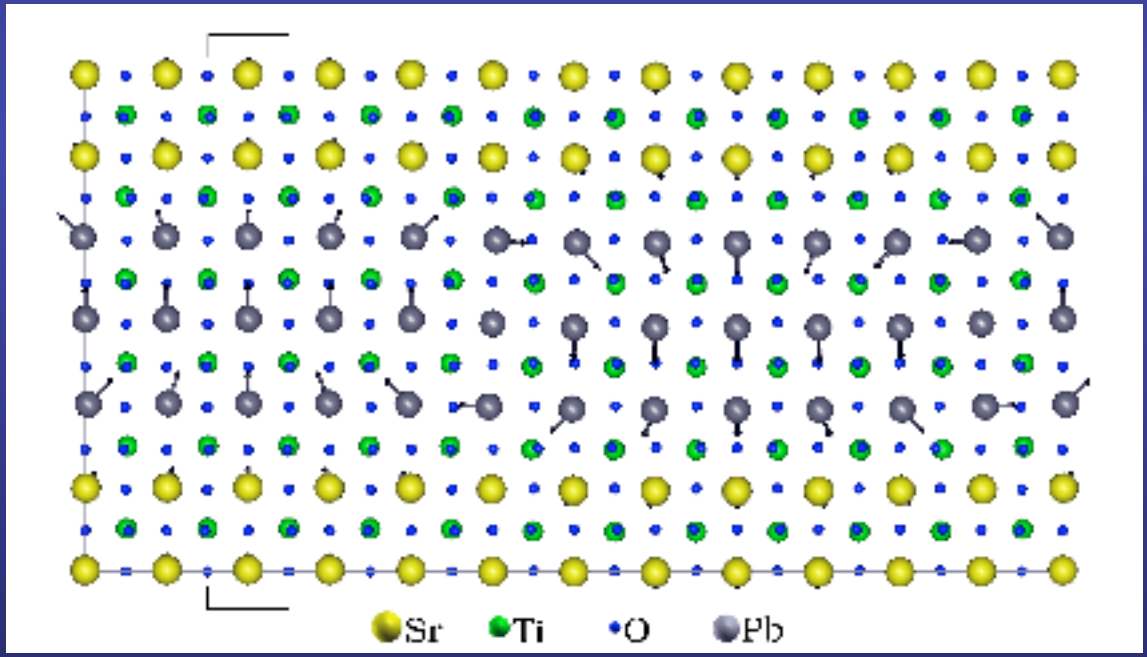
Domains in $PbTiO_3/SrTiO_3$ (3/3) superlattices: vortices in larger domain periodicities

(3,3) superlattice

12 unit cells of domain periodicity

Fully relaxed

	w/o AFD	with AFD
P^{PTO} (μC/cm²)	(0, 0, 62)	(0, 2, 55)
P^{STO} (μC/cm²)	(0, 0, 32)	(0, 0, 30)



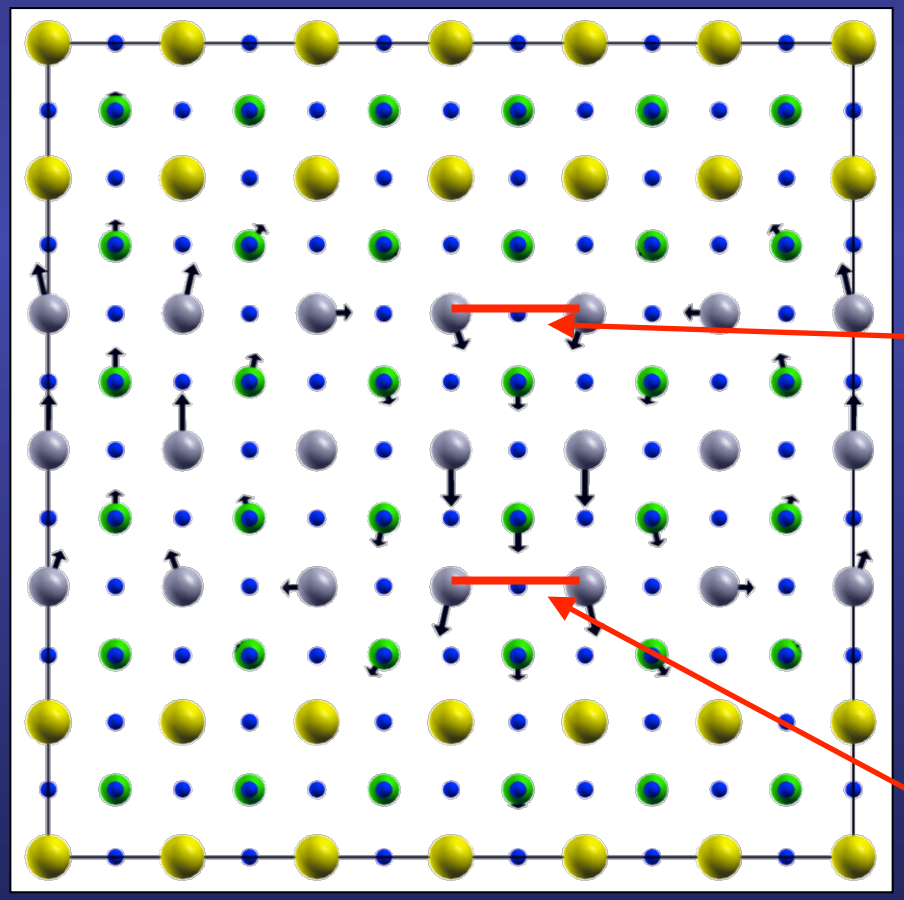
Large in-plane displacements for the Pb ~ 0.2 Å → TEM experiment?

Domains in $PbTiO_3/SrTiO_3$ superlattices: domain structure induces inhomogeneous strain

(3,3) superlattice

6 unit cells of domain periodicity

Fully relaxed



Polarization domains → good screening

	w/o AFD	with AFD
P^{PTO} (μC/cm²)	(0, 0, 68)	(0,26,56)
P^{STO} (μC/cm²)	(0, 0, 25)	(0,1,23)

Domains induce large strain gradient

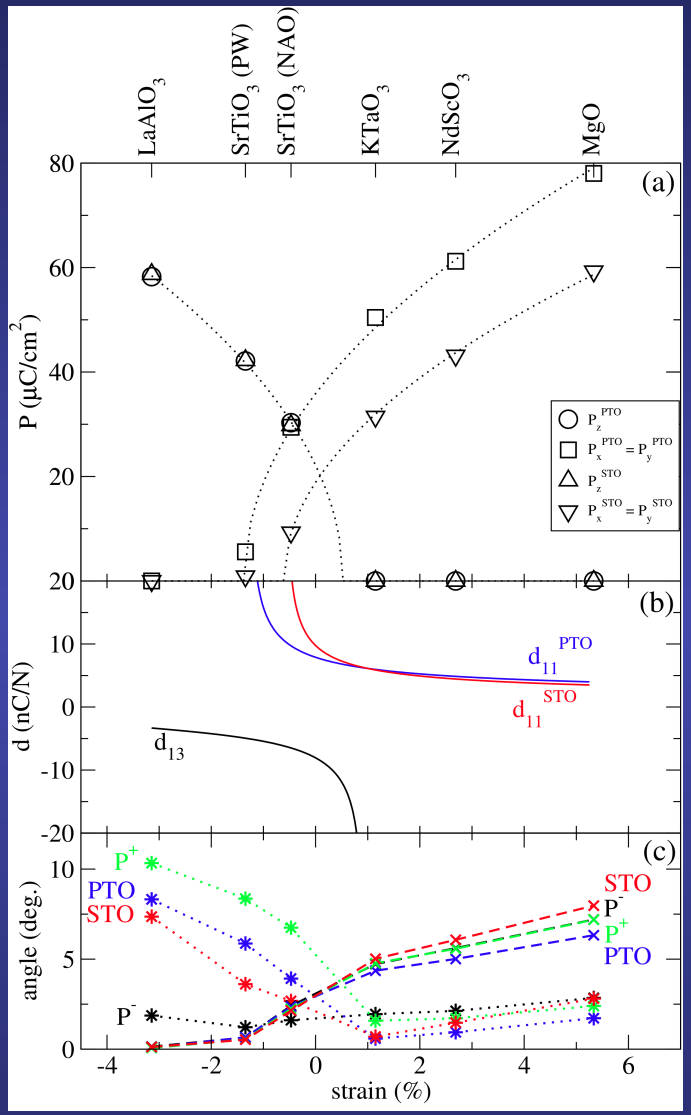
$a_{\text{PTO down}} = 3.76$ Å

$\Delta a = 0.20$ Å

$a_{\text{PTO up}} = 3.97$ Å

$$\frac{\partial \varepsilon_{11}}{\partial z} = 6.8 \times 10^{7}\ \text{m}^{-1}$$

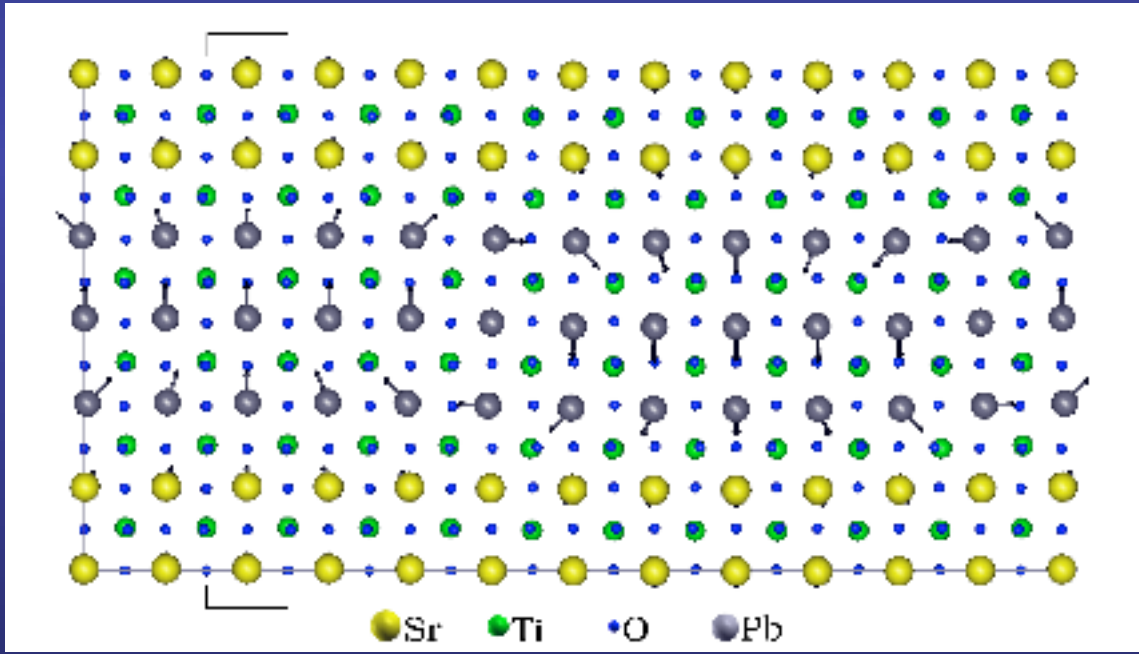
Conclusions



Mixed ferroelectric-antiferrodistortive-strain coupling in $PbTiO_3/SrTiO_3$ superlattices

Electrostatic and covalent origin

Large electromechanical response around the strain imposed by a $SrTiO_3$ lattice constant

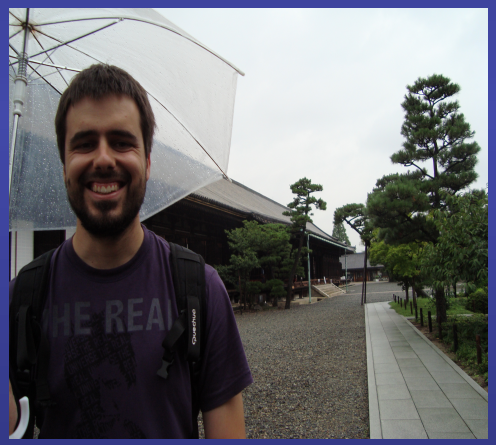


Close competition between monodomain and closure-domain structures

Many thanks to

Pablo García-Fernández

Pablo Aguado-Puente



Finantial support

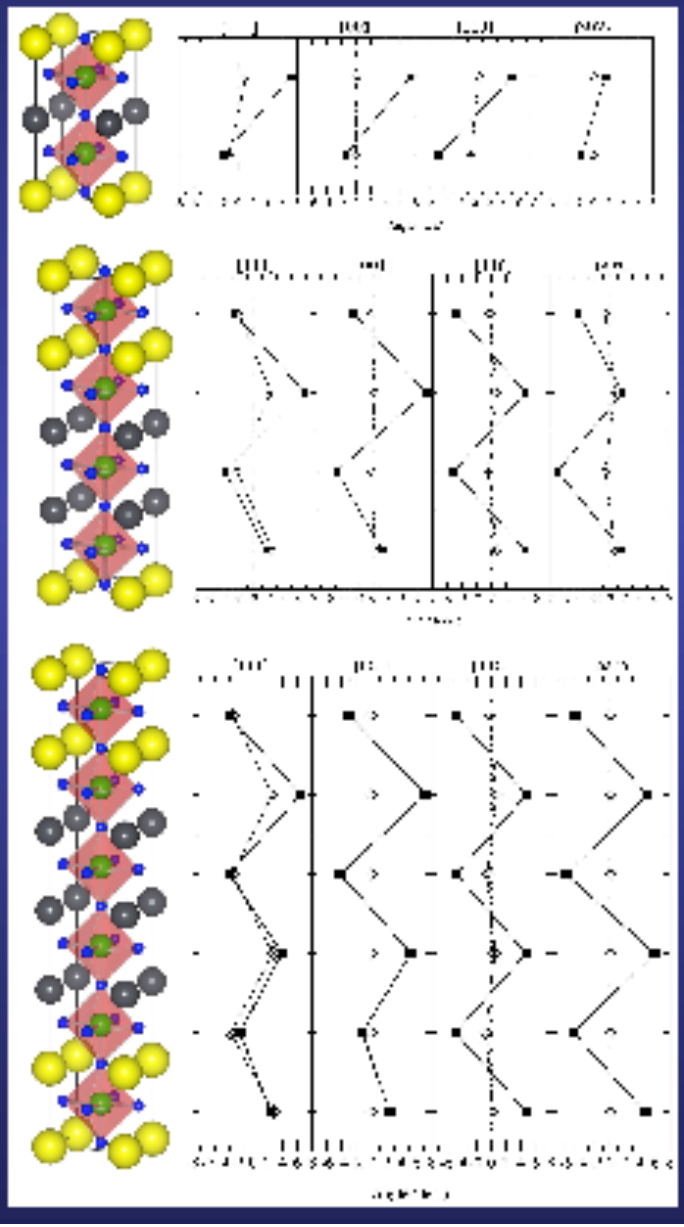
Engineering Exotic Phenomena
Ox/Des
at Oxide Interfaces

Computer time

RES
RED ESPAÑOLA DE SUPERCOMPUTACIÓN

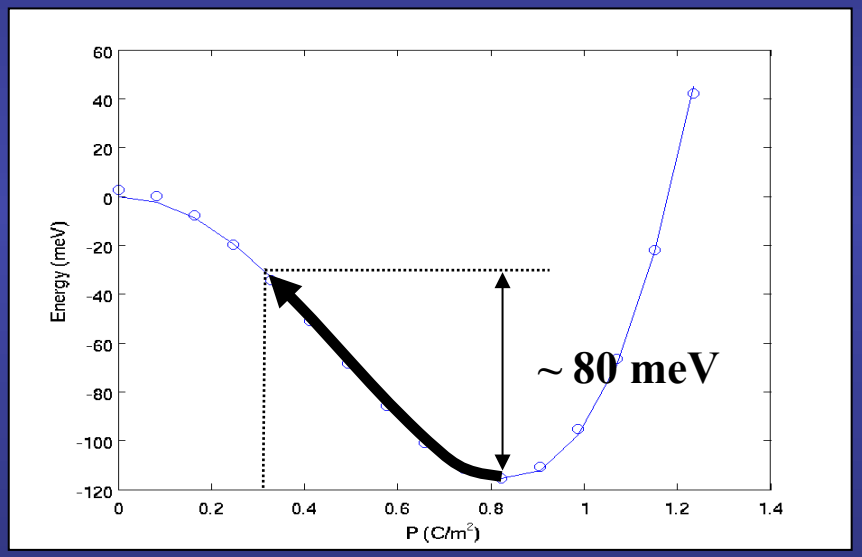
More info …

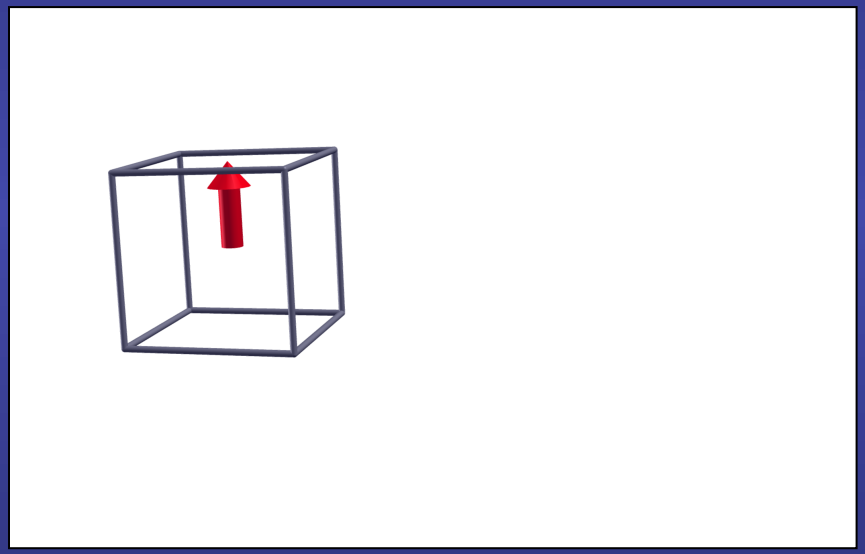
Monodomain $PbTiO_3/SrTiO_3$ superlattices with different periodicities



Origin of the *r*-phase: $PbTiO_3$ prefers to rotate over a reduction of the out-of-plane-polarization

Double-well curve of bulk tetragonal PbTiO3





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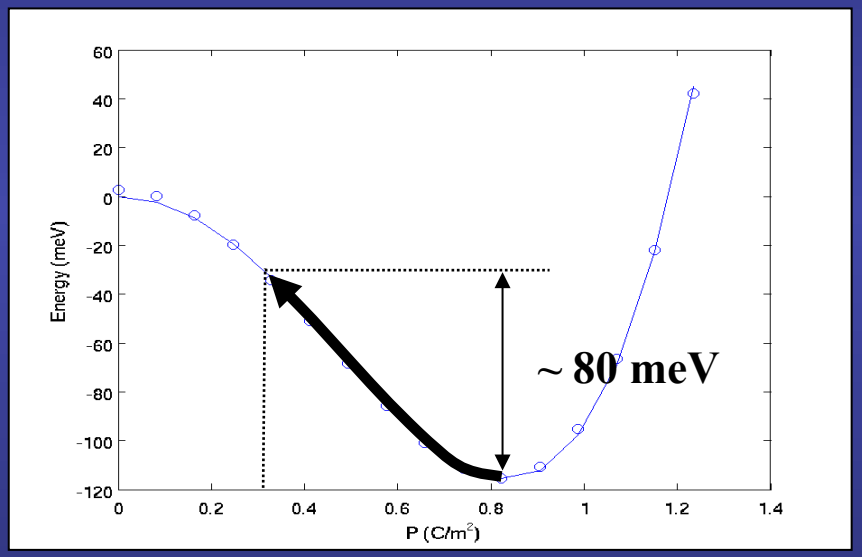
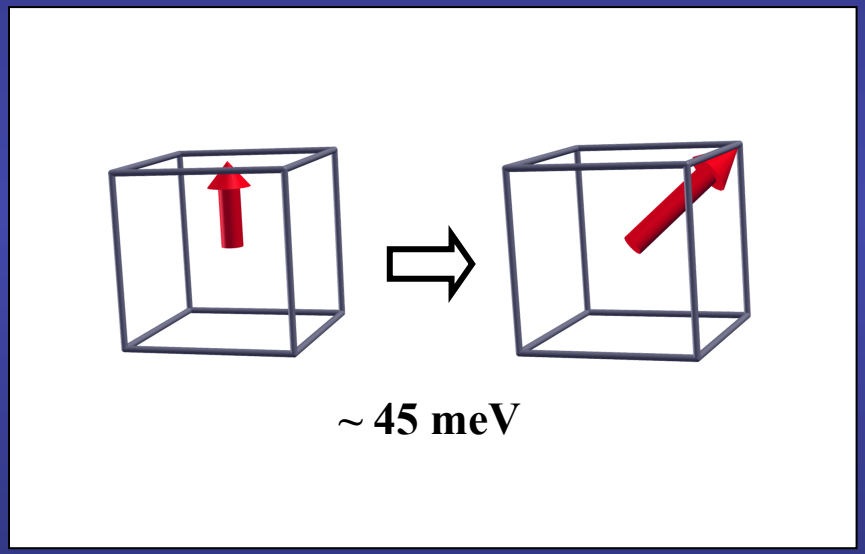
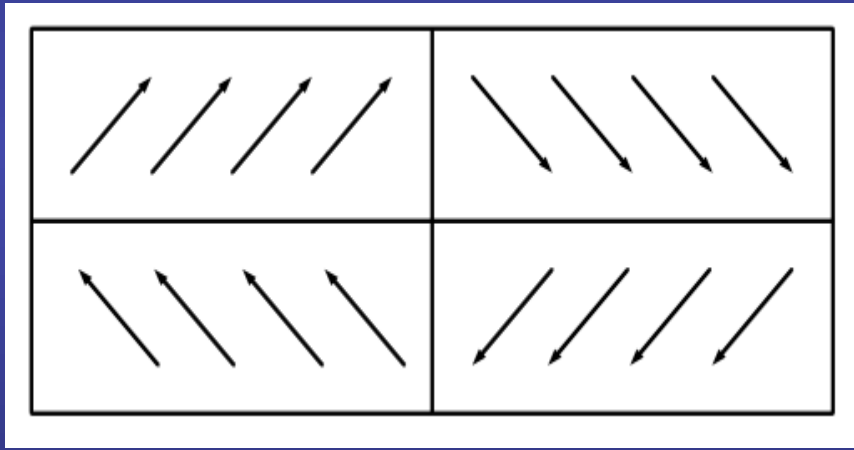


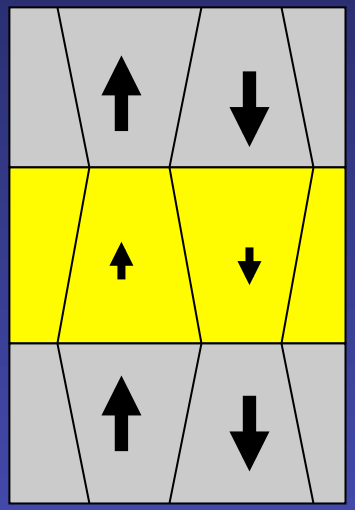


Its actually *cheaper* to rotate!

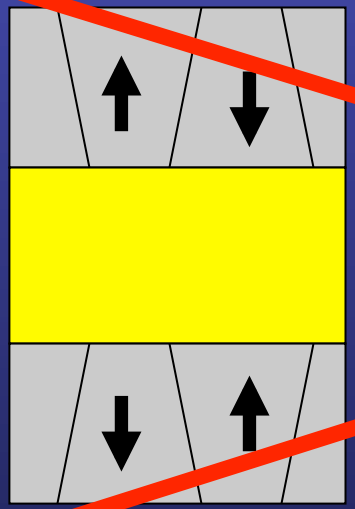
No polarization along x



Elastic vs electrostatic interlayer coupling



- Domains induce large strain gradient
- Related with flexoelectricity, face where cation move towards expands.
- STO is forced to distort the opposite way → elastic cost

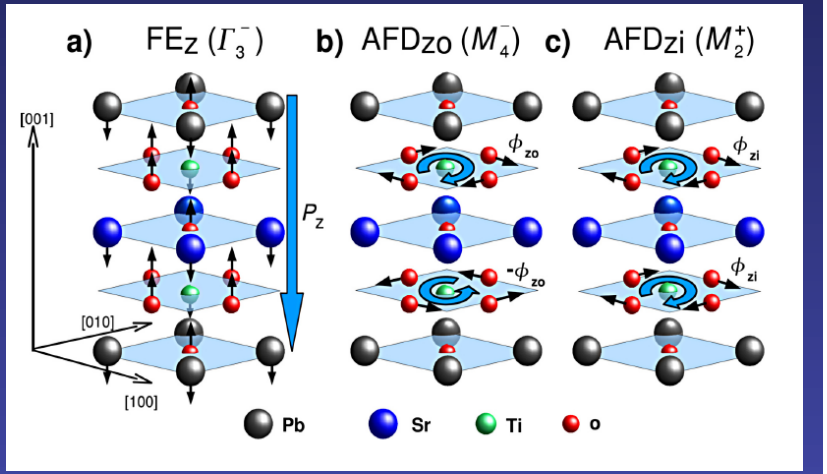


- Minimization of elastic energy?
- Greater electrostatic cost
- Minimization of elastic energy?

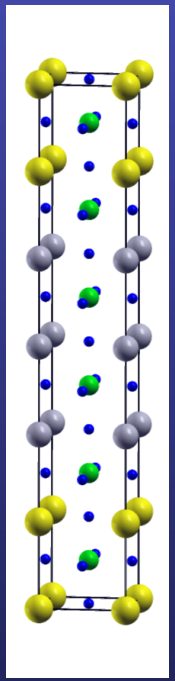
Simulation of monodomain $PbTiO_3/SrTiO_3$ superlattices

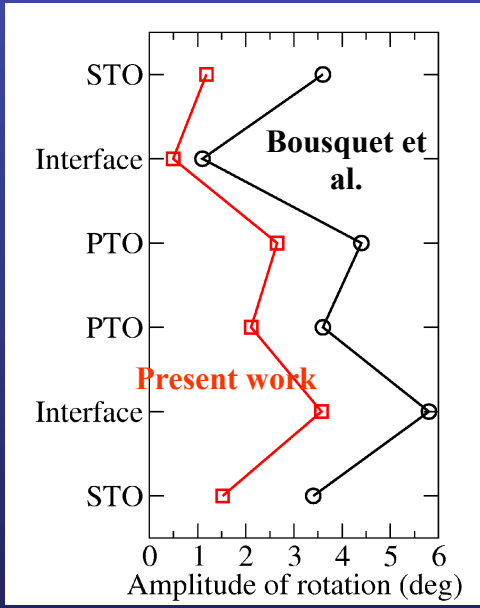
Bousquet et al., Nature 452, 732 (2008)

- Monodomain configuration
- Strong coupling between FE and AFD modes
- Improper FE
- Larger periodicities → Interfacial effect

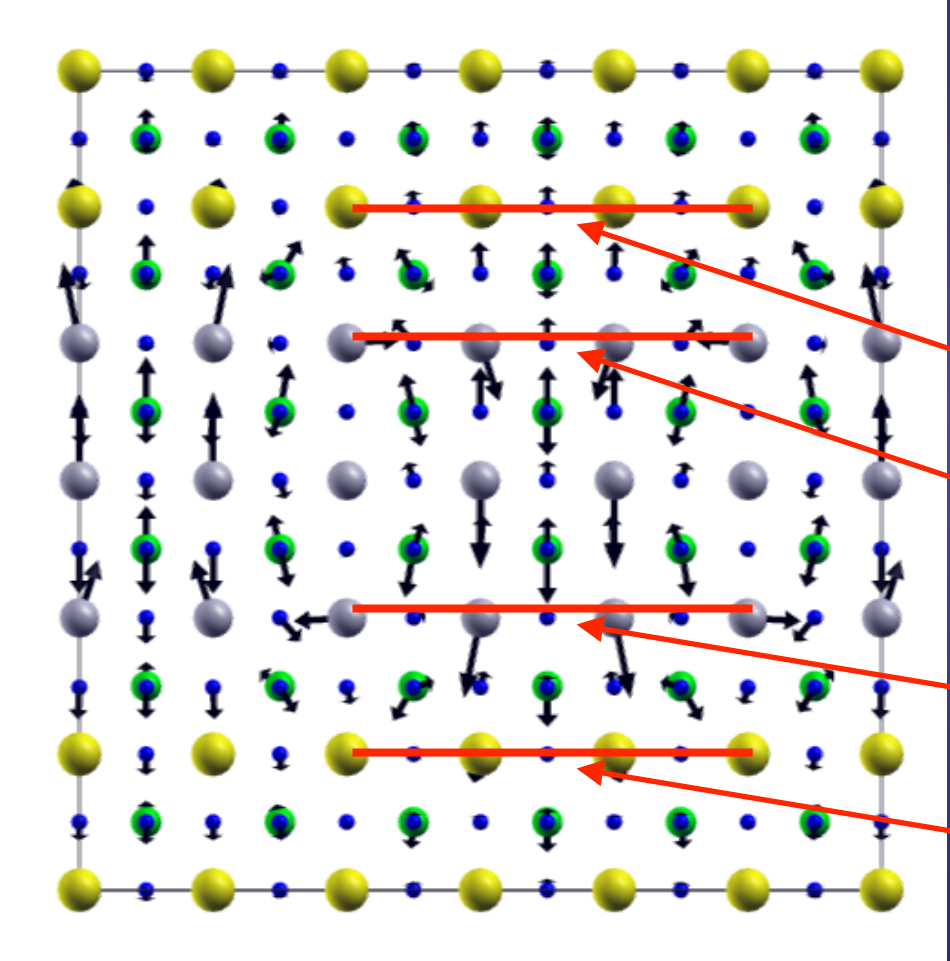


(3,3) superlattices:





Inhomogeneous distortion in $SrTiO_3$ /$PbTiO_3$ superlattices



Domain widths:

$a_{STO\ bulk} = 3.874$ Å

$w_{STO\ up} = 11.56 = 3 \times 3.85$ Å

$w_{PTO\ down} = 11.32 = 3 \times 3.77$ Å

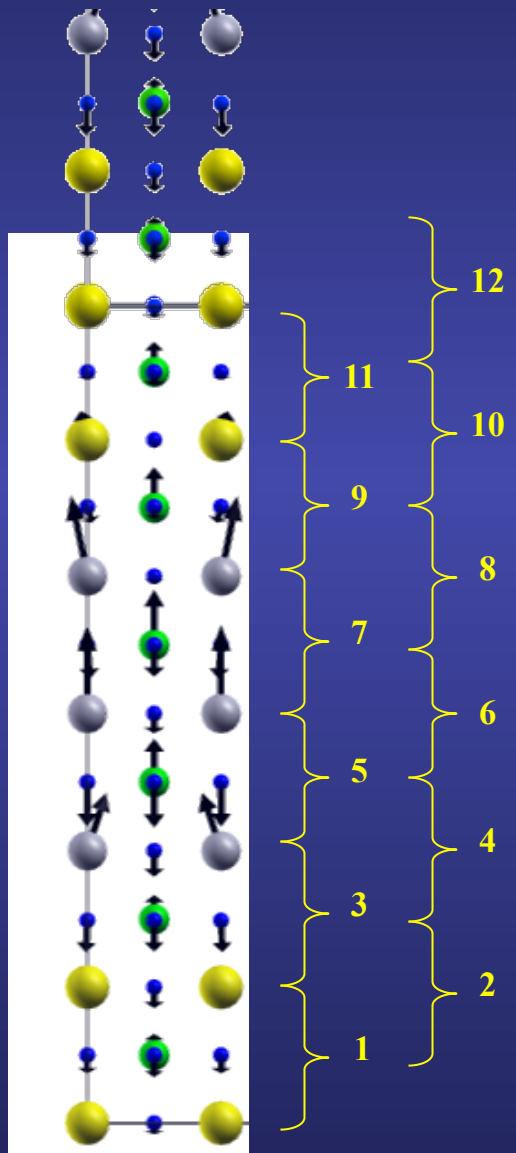
$w_{PTO\ up} = 11.92 = 3 \times 3.97$ Å

$w_{STO\ down} = 11.68 = 3 \times 3.89$ Å

$\Delta w_{STO} = 0.12$ Å

$\Delta w_{PTO} = 0.60$ Å

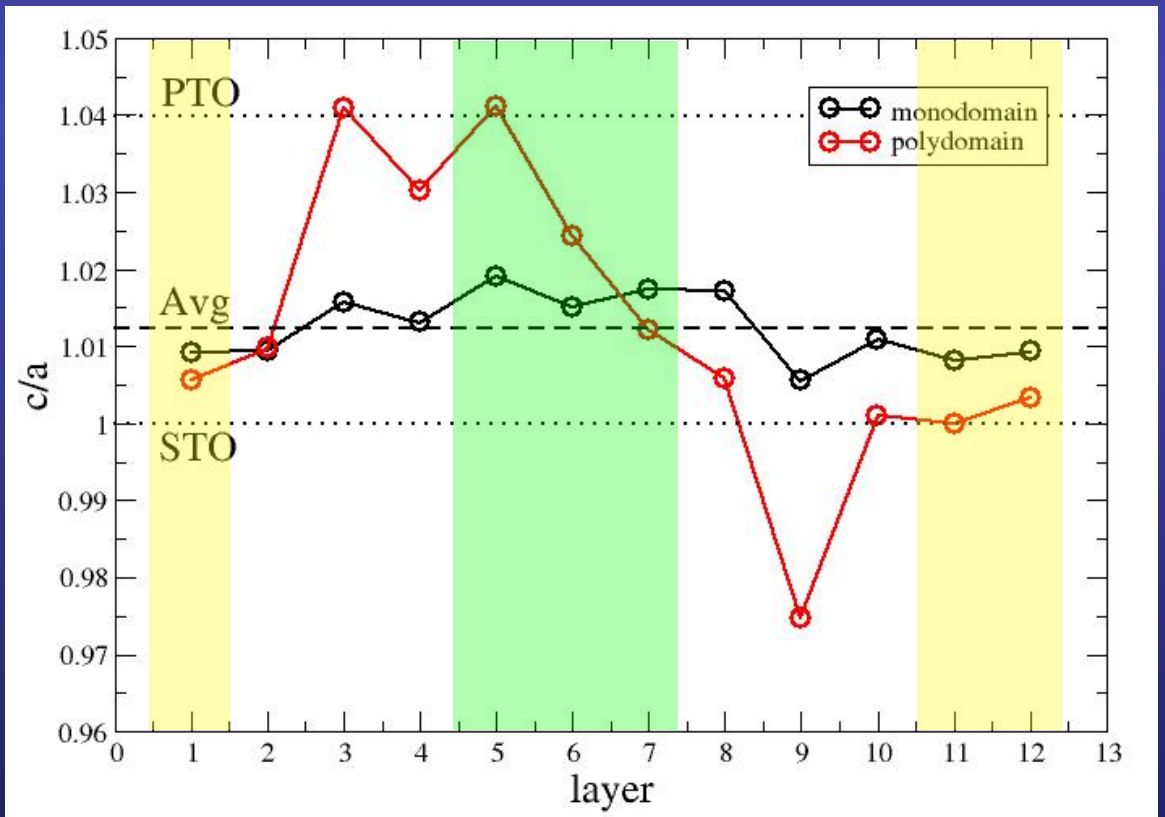
Tetragonality in polydomain $SrTiO_3$ /$PbTiO_3$ superlattices



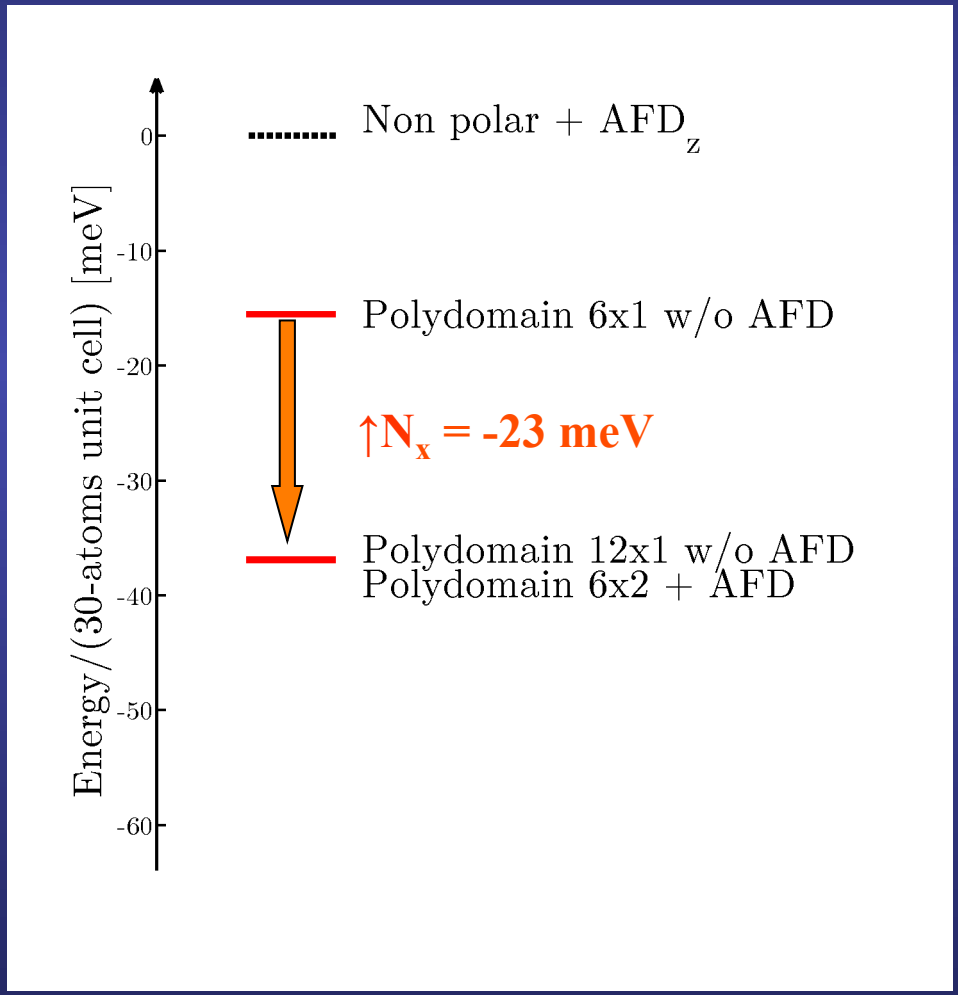
Out of plane lattice parameters:

$c_{STO\ bulk}$ = 3.874 Å

$c_{PTO\ bulk}$ = 4.025 Å



PTO/STO superlattices: relative stability of monodomain and polydomain configurations

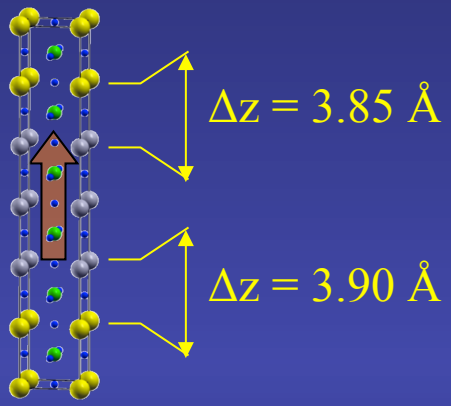


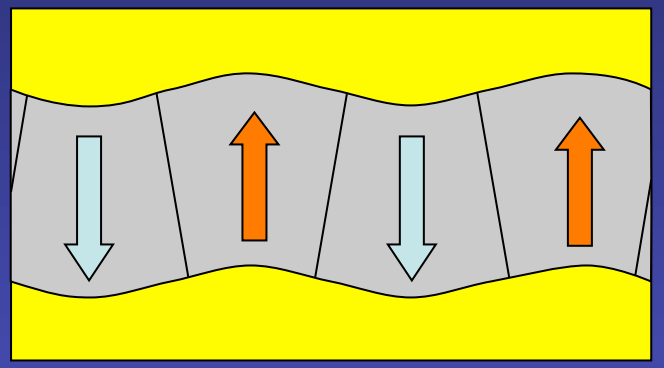
- AFD instabilities increase stability
- Domain periodicity ~ 12 unit cells

  (experiment ~ 11 unit cells)

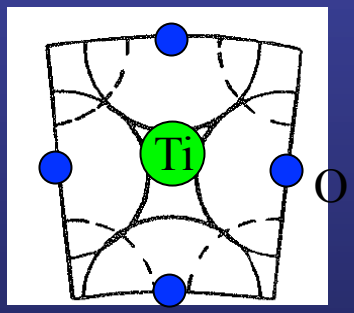
Inhomogeneous strain due to domain structure in PTO/STO

• Polarization breaks inversion symmetry → different bonding at up and down interfaces and diffetent interfacial distance.





• Flexoelectric effect? → unit cell side where cations move towards, expands.



• Large flexoelectric effect observed in FE materials.

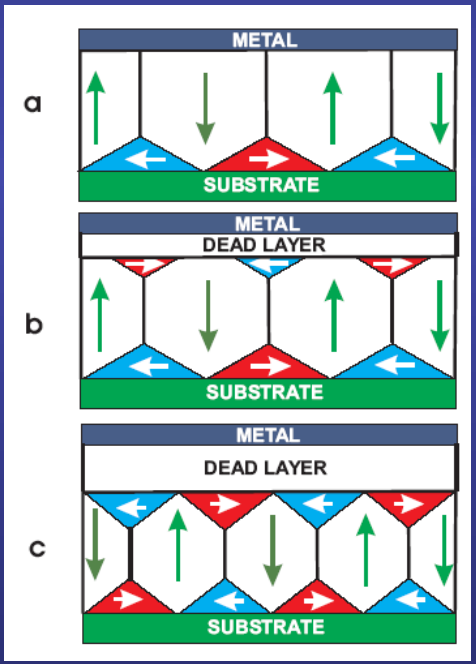
• Spontaeous P induces spontaneous strain gradient.

Bursian et al., Fiz. Tv. Tela 10, 1413 (1968)

Domains of closure recently predicted using a model hamiltonian approach

48 Å thick $PbZr_{0.4}Ti_{0.6}O_3$ thin films

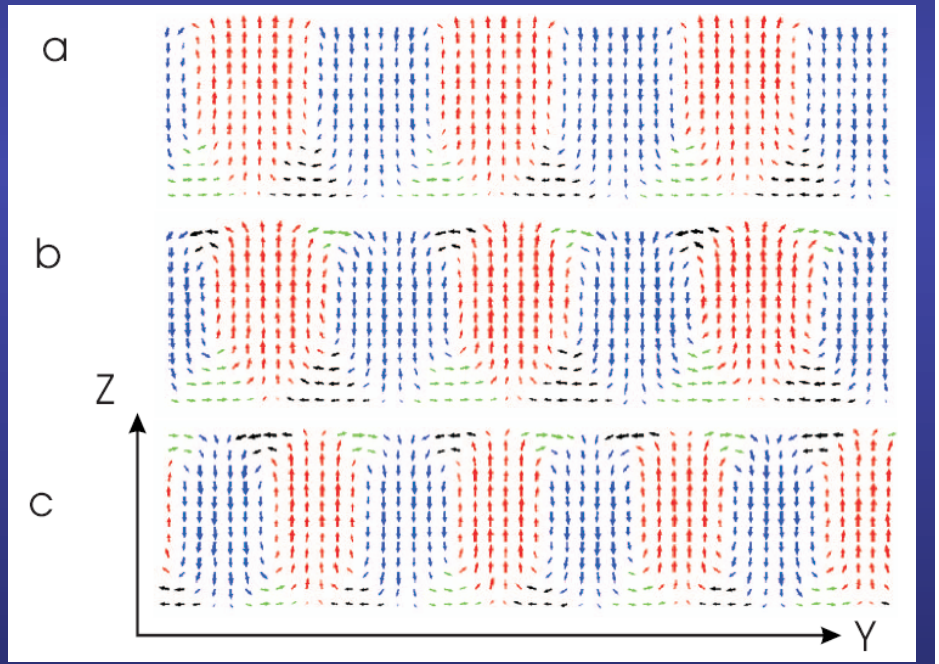
sandwiched with a nongrounded metallic plate (top) and a non-conductive substrate (bottom)



d = 0

d = 0.3 a

d = 0.5 a



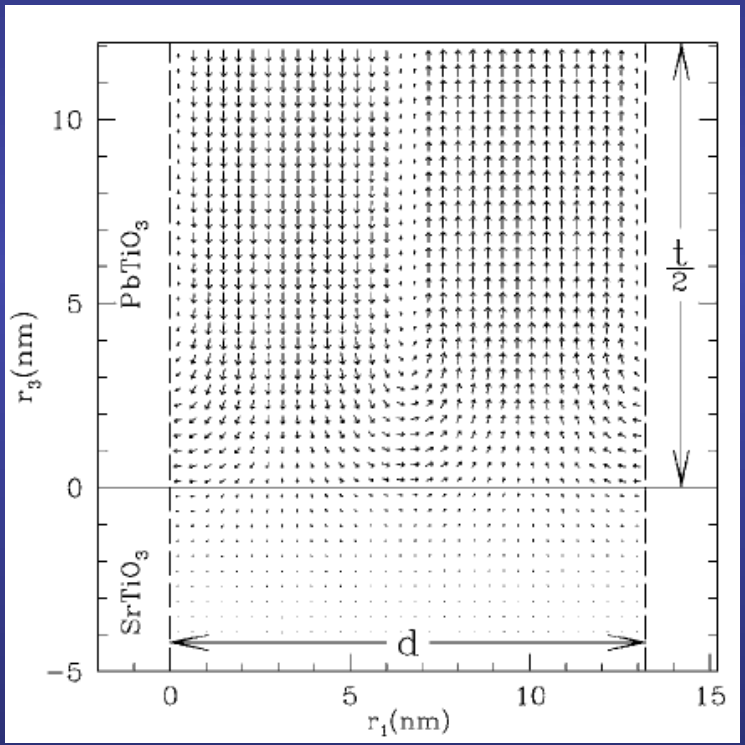
Dead layer thickness

S. Prosandeev and L. Bellaiche, Phys. Rev. B 75, 172109 (2007)

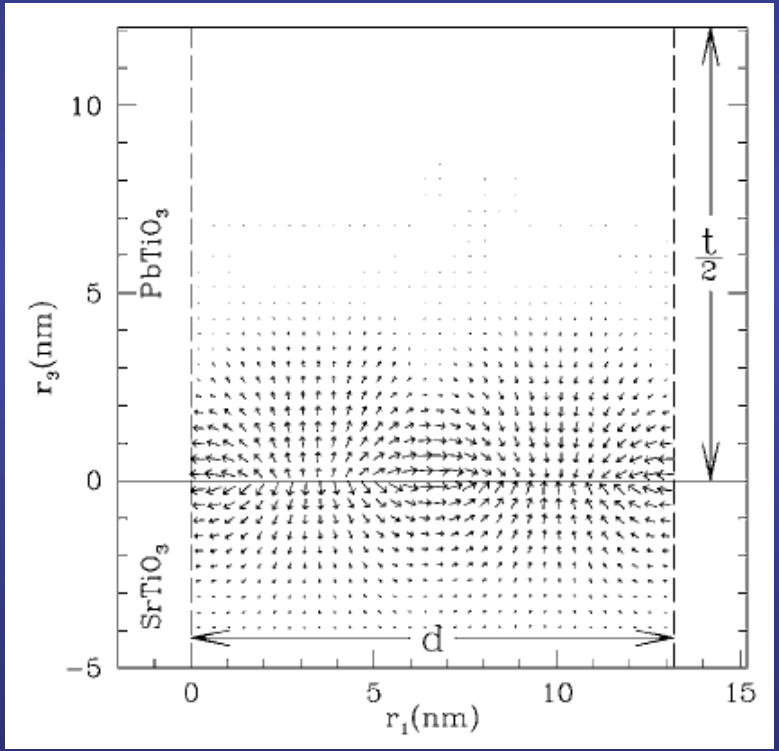
Domains of closure recently predicted using a phenomenological thermodynamic potential

242 Å thick $PbTiO_3$ thin films

sandwiched with a nonconducting $SrTiO_3$ electrodes @ 700 K stripe period 132 Å



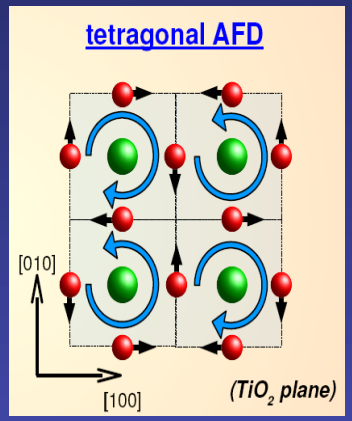
Polarization distribution



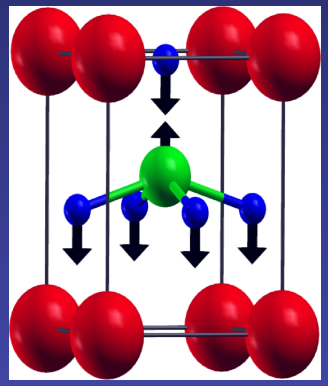
Equilibrium field distribution

G. B. Stephenson and K. R. Elder, J. Appl. Phys. 100, 051601 (2006)

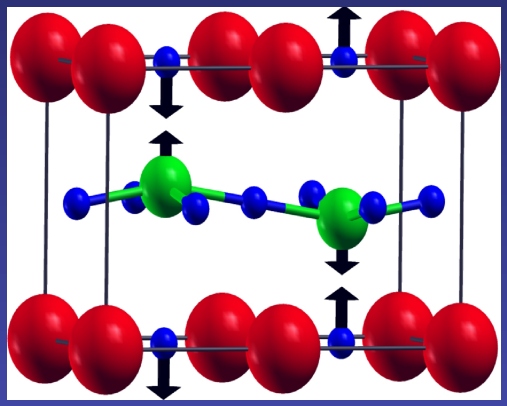
ABO_3 perovskite structure exhibits several lattice instabilities. Competition between polar and non polar instabilities.



Antiferrodistortive

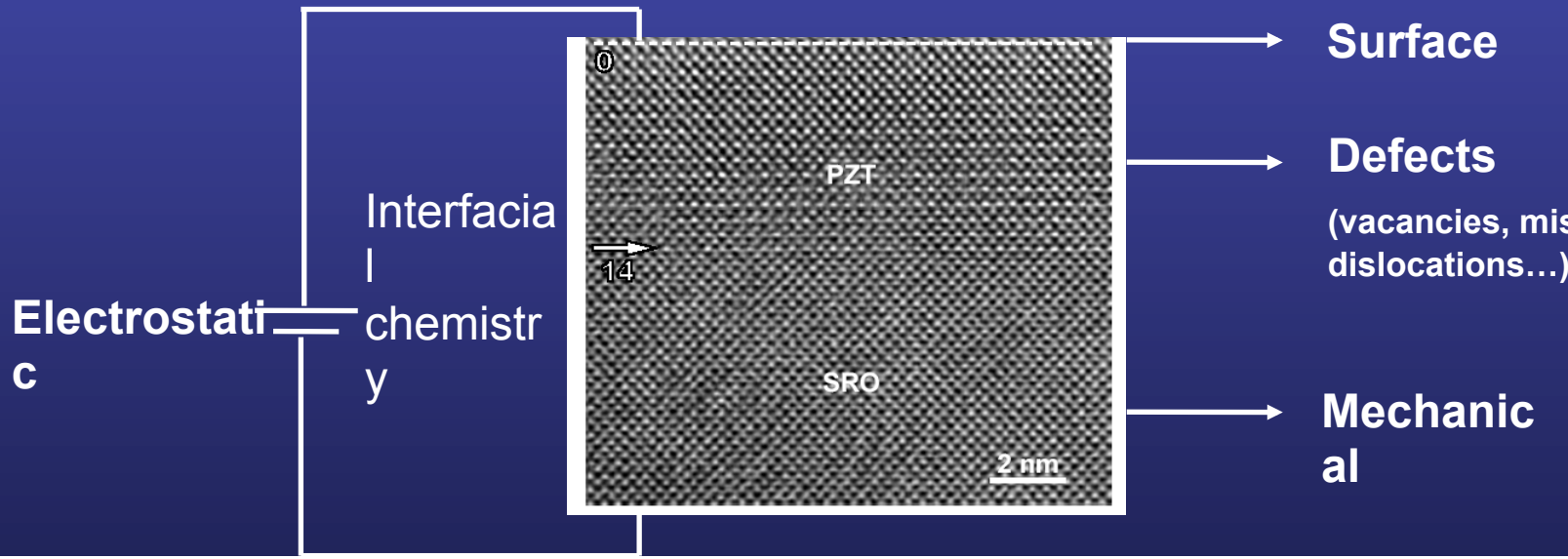


Ferroelectric



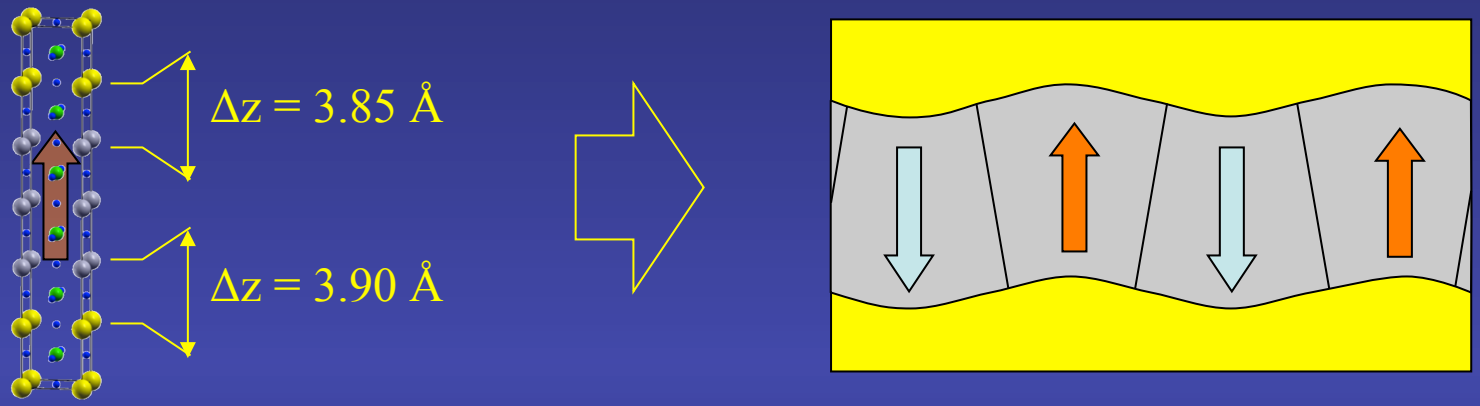
Antiferroelectric

Balance might be altered in nanostructures

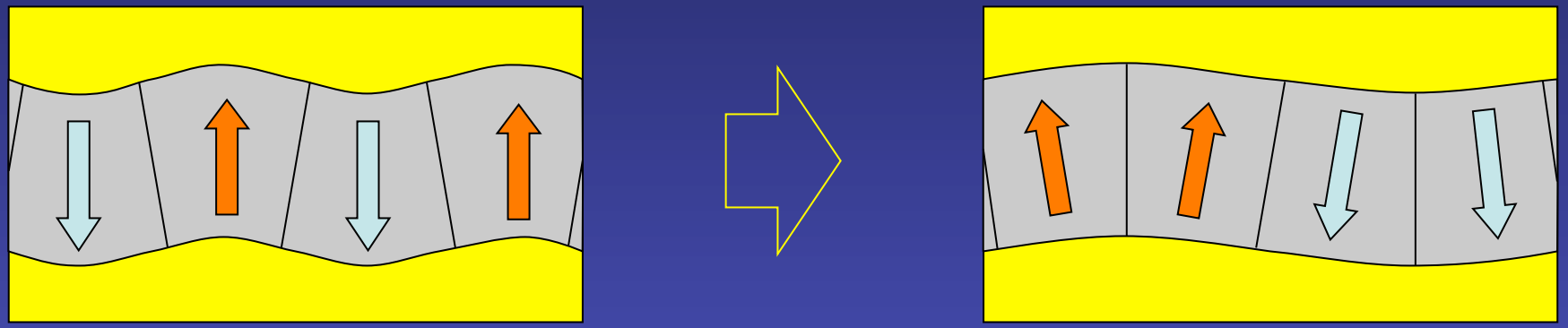


Inhomogeneous strain due to domain structure in $PbTiO_3/SrTiO_3$ superlattices

Polarization breaks inversion symmetry → different bonding at up and down interfaces and diffetent interfacial distance.



Elastic energy associated with inhomogeneous strain play a role in domain structure



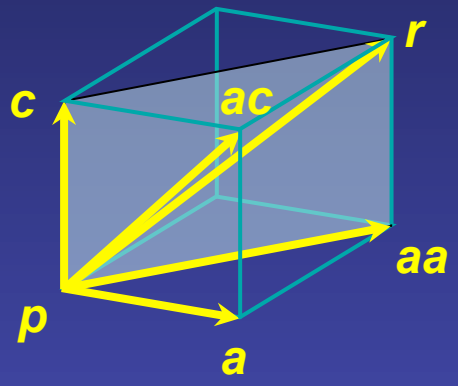
Balance:

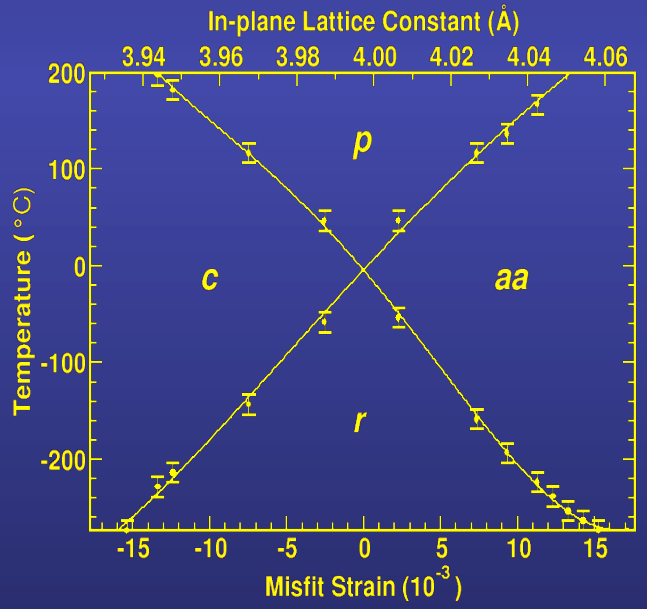
Elastic energy ↔ Electrostatic energy ↔ Domain wall energy

Domain wall interaction more complex than in bulk/thick films

Need for a model

Common wisdom: epitaxial $BaTiO_3$ under compressive in-plane strain stabilizes the tetragonal phase, with enhancement of P_s

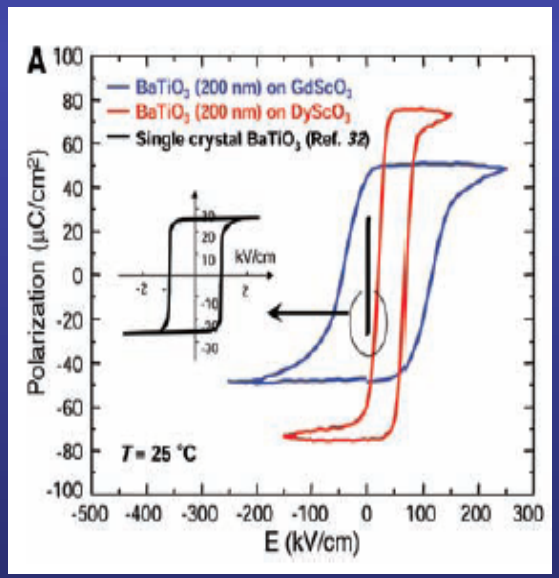




O. Diéguez *et al.*, Phys. Rev. B 69, 212101 (2004)

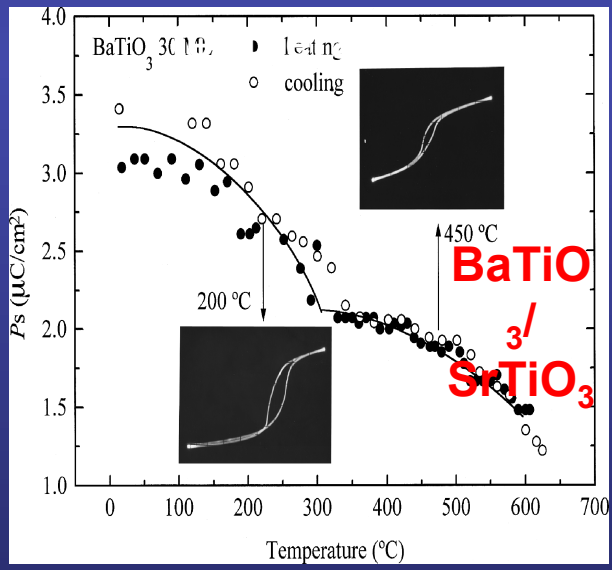
B. Lai *et al.*, Appl. Phys. Lett. 86, 132904 (2005)

Enhancement of the remnant polarization



K. J. Choi *et al.*, Science 306, 1005 (2004)

Enhancement of the transition



Yoneda *et al.*, J. Appl. Phys. 83, 2458 (1998)

Simulation of monodomain $PbTiO_3/SrTiO_3$ (3/3) superlattices

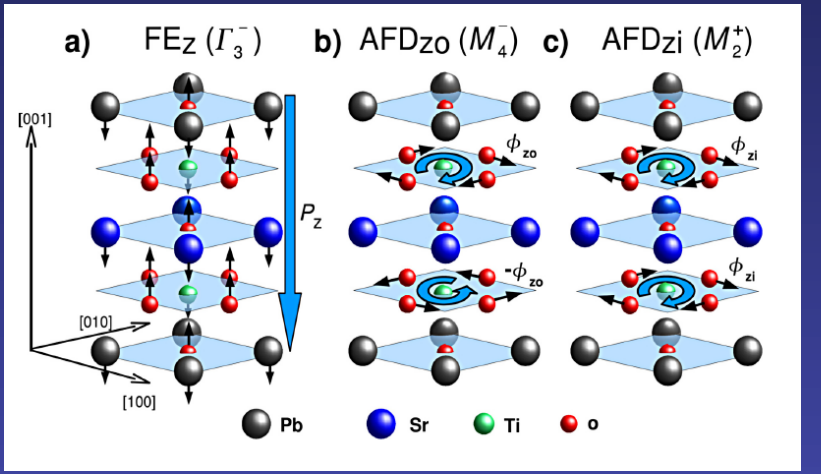
Bousquet *et al.*, Nature 452, 732 (2008)

Monodomain configuration

Strong coupling between FE and AFD modes

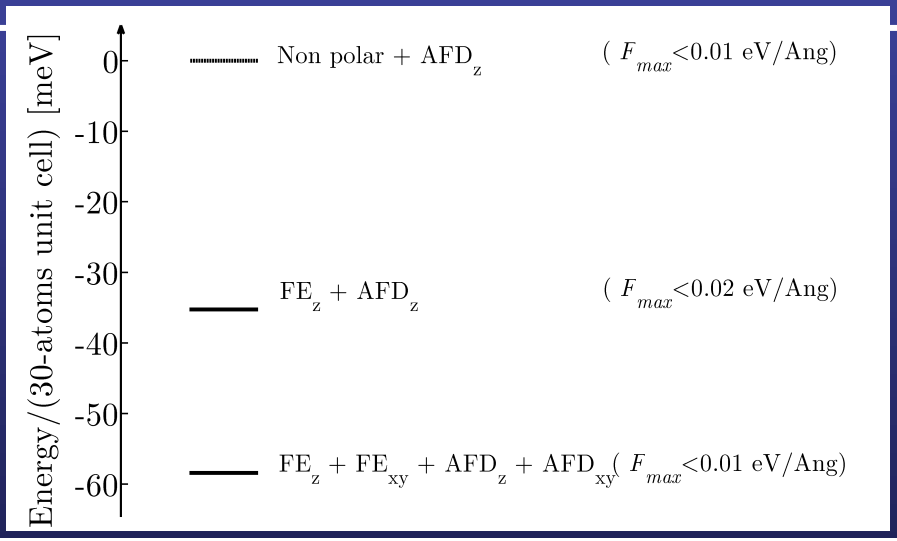
Improper FE for the short-period superlattices

Larger periodicities → Interfacial effect



$[PbTiO_3]_3/[SrTiO_3]_3$ = (3,3) superlattices:

	Bousquet *et al.*	Present work
Ground state	$FE_z + AFD_z$	$FE_z + FE_{xy} + AFD_z + AFD_{xy}$



-24 meV

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Bousquet *et al.*, Nature 452, 732 (2008)

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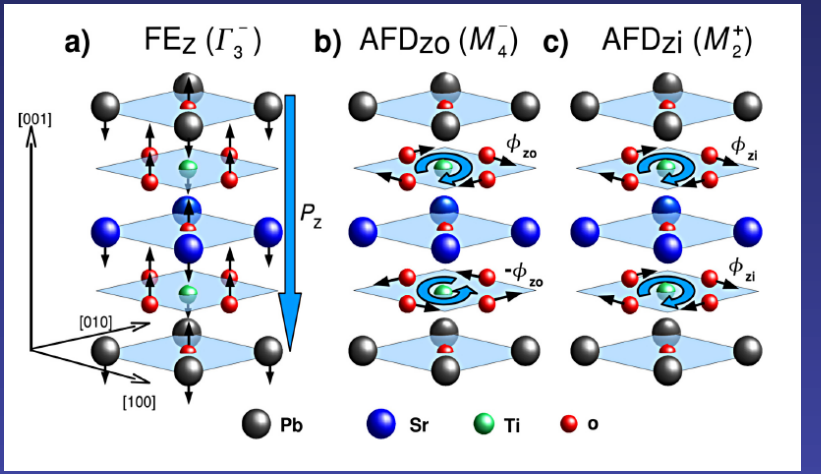

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P^{STO} (μC/cm²)	(0, 0, 37.5)	(5, 5, 29)
P^{PTO} (μC/cm²)	(0, 0, 35.8)	(36, 32, 31)

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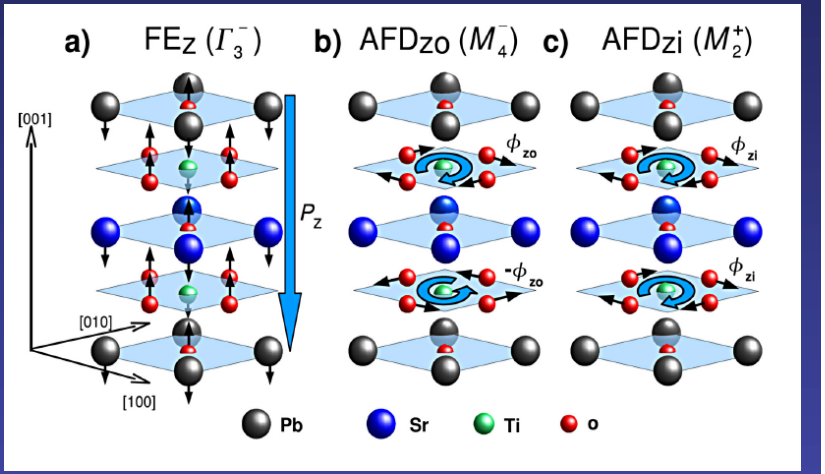

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P^{PTO} (μC/cm²)	(0, 0, 35.8)	(36, 32, 31)
Strain of PTO on STO	-1.2%	-0.5%

FE ↔ AFD coupling is extremely sensitive to strain!

Simulation of monodomain $PbTiO_3/SrTiO_3$ (3/3) superlattices

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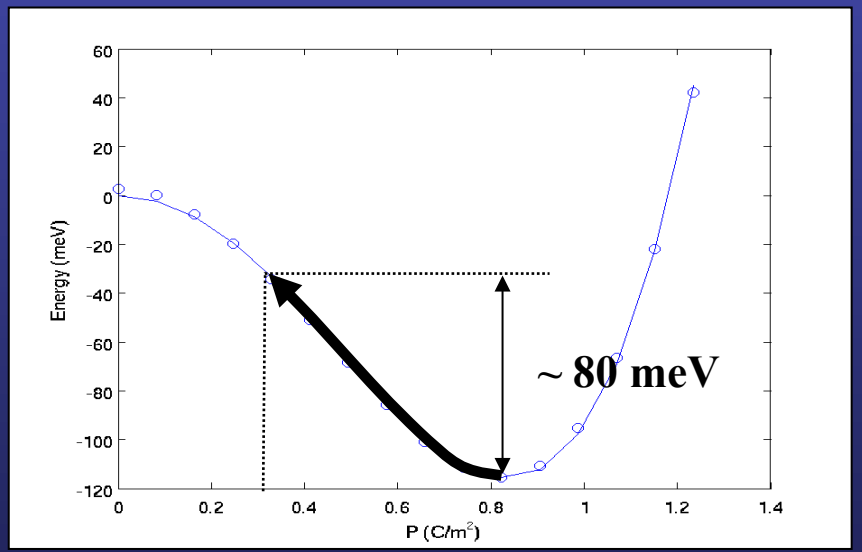
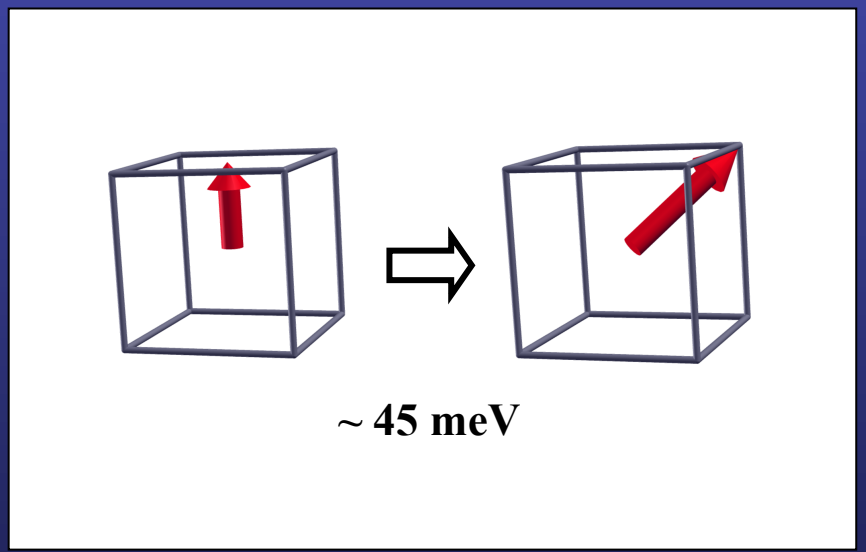
	Present work
Ground state	$FE_z + FE_{xy} + AFD_z + AFD_{xy}$
P^{STO} (μC/cm²)	(5, 5, 29)
P^{PTO} (μC/cm²)	(36, 32, 31)

Why $PbTiO_3$ polarizes in-plane?

Its actually *cheaper* to rotate!





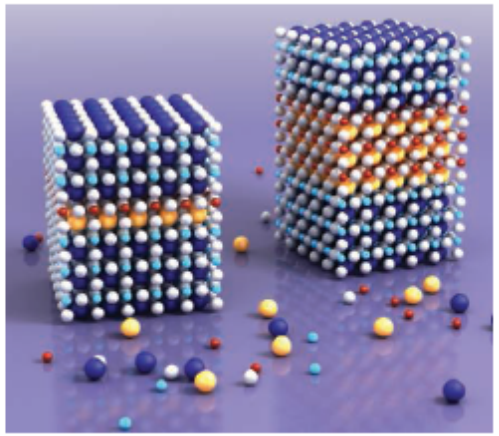
Recent discoveries on transition metal oxides: one of the "top tens" scientific breakthroughs of 2007

Breakthrough of the Year

5 BEYOND SILICON? Sixty years ago, semiconductors were a scientific curiosity. Then researchers tried putting one type of semiconductor up against another, and suddenly we had diodes, transistors, microprocessors, and the whole electronic age. Startling results this year may herald a similar burst of discoveries at the interfaces of a different class of materials: transition metal oxides.

Transition metal oxides first made headlines in 1986 with the Nobel Prize–winning discovery of high-temperature superconductors. Since then, solid-state physicists keep finding unexpected properties in these materials—including colossal magnetoresistance, in which small changes in applied magnetic fields cause huge changes in electrical resistance. But the fun should really start when one oxide rubs shoulders with another.

If different oxide crystals are grown in layers with sharp interfaces, the effect of one crystal structure on another can shift the positions of atoms at the interface, alter the population of electrons, and even change how



Tunable sandwich. In lanthanum aluminate sandwiched between layers of strontium titanate, a thick middle layer (*right*) produces conduction at the lower interface; a thin one does not.

Science, 318, 1846 (2007)

The field is still in an incipient stage, comparable to that of semiconductors 60 years ago

PERSPECTIVES

PHYSICS

When Oxides Meet Face to Face

Elbio Dagotto

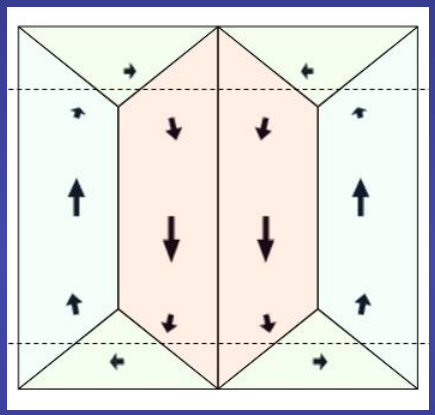
Despite recent activity, the field of oxide interfaces remains virtually unexplored. What might happen if we could mix materials with vastly different properties such as ferromagnets, antiferromagnets, superconductors, ferroelectrics, multiferroics, geometrically frustrated spin systems, heavy fermions, and others? Considering this enormous number of

Polydomain phases in ferrolectric nanocapacitors adopt the form of a “domain of closure”, common in ferromagnets

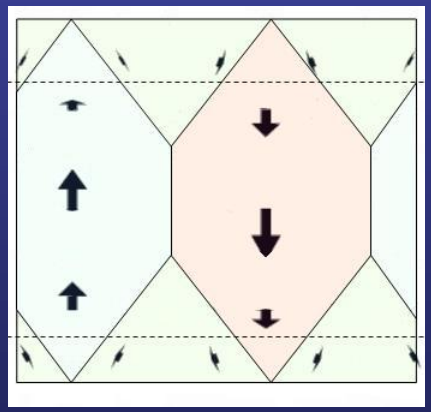
2-unit-cells thick $BaTiO_3$ layer in between $SrRuO_3$ electrodes

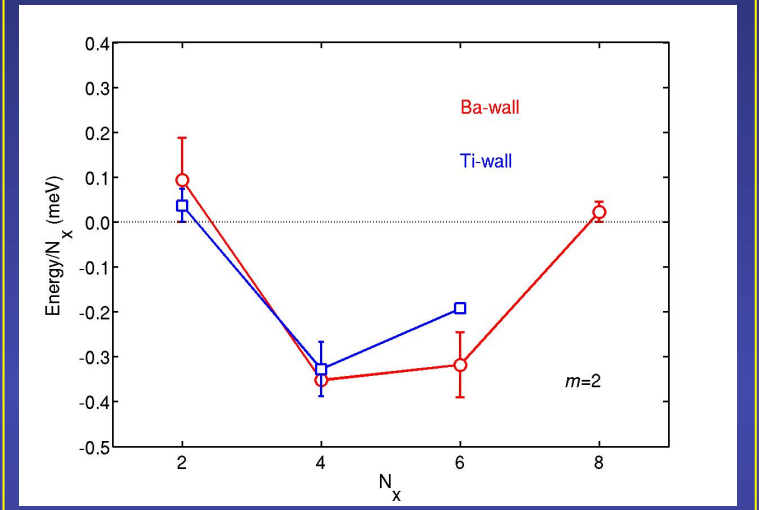
N_x=4

BaO wall

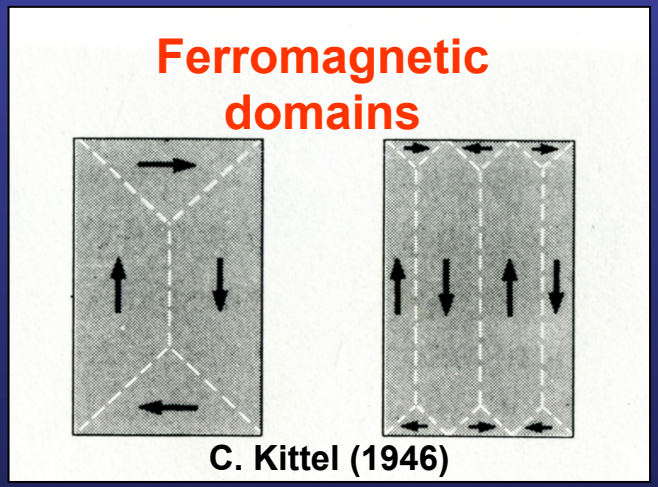


TiO_2 wall



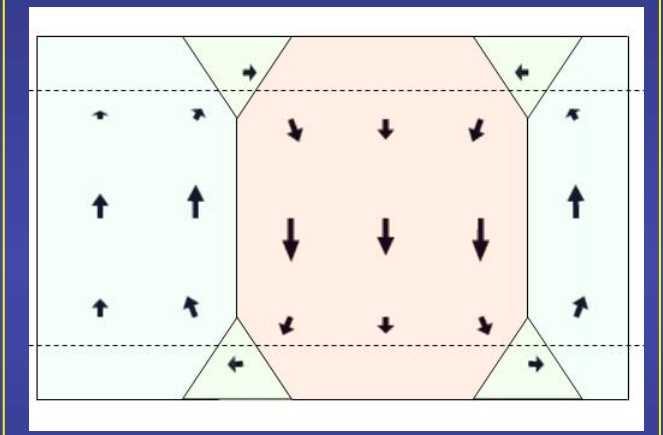


P. Aguado-Puente and J. Junquera
Phys. Rev. Lett. 100, 177601 (2008)

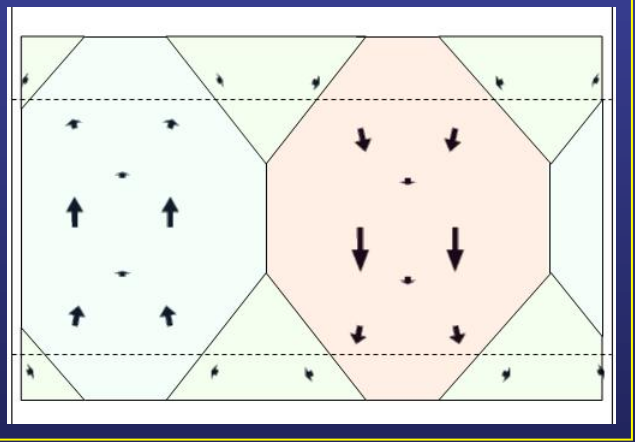


N_x=6

BaO wall

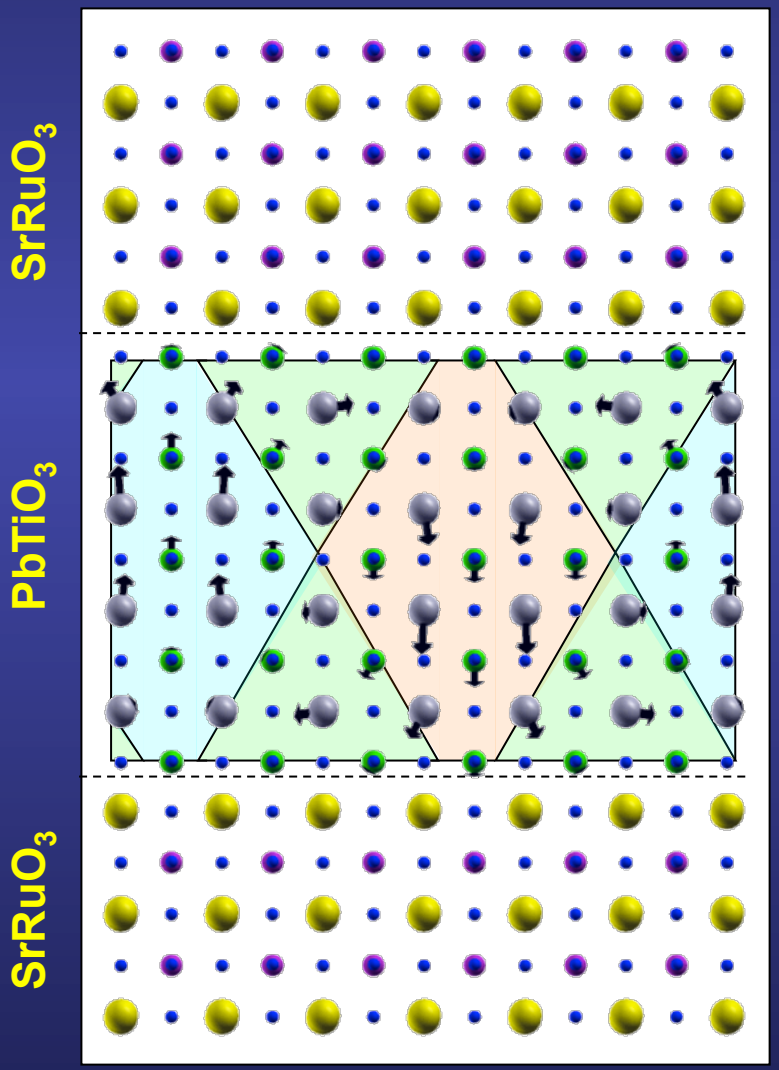


TiO_2 wall



Domains of closure in $PbTiO_3/SrRuO_3$ capacitors from first-principles

C. Lichtensteiger *et al.*
"Oxide ultrathin films: science and technology"
Ed. by G. Pacchini and S. Valeri (Wiley, 2011)



Short-circuit

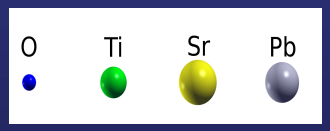
4-unit-cell thick $PbTiO_3$

6 unit cells of domain periodicity

Fully relaxed

P = 65 μC/cm² → good screening

Vortices at DW ↔ Domains of closure
(but in this case, closed by the displacements of the Pb atoms)

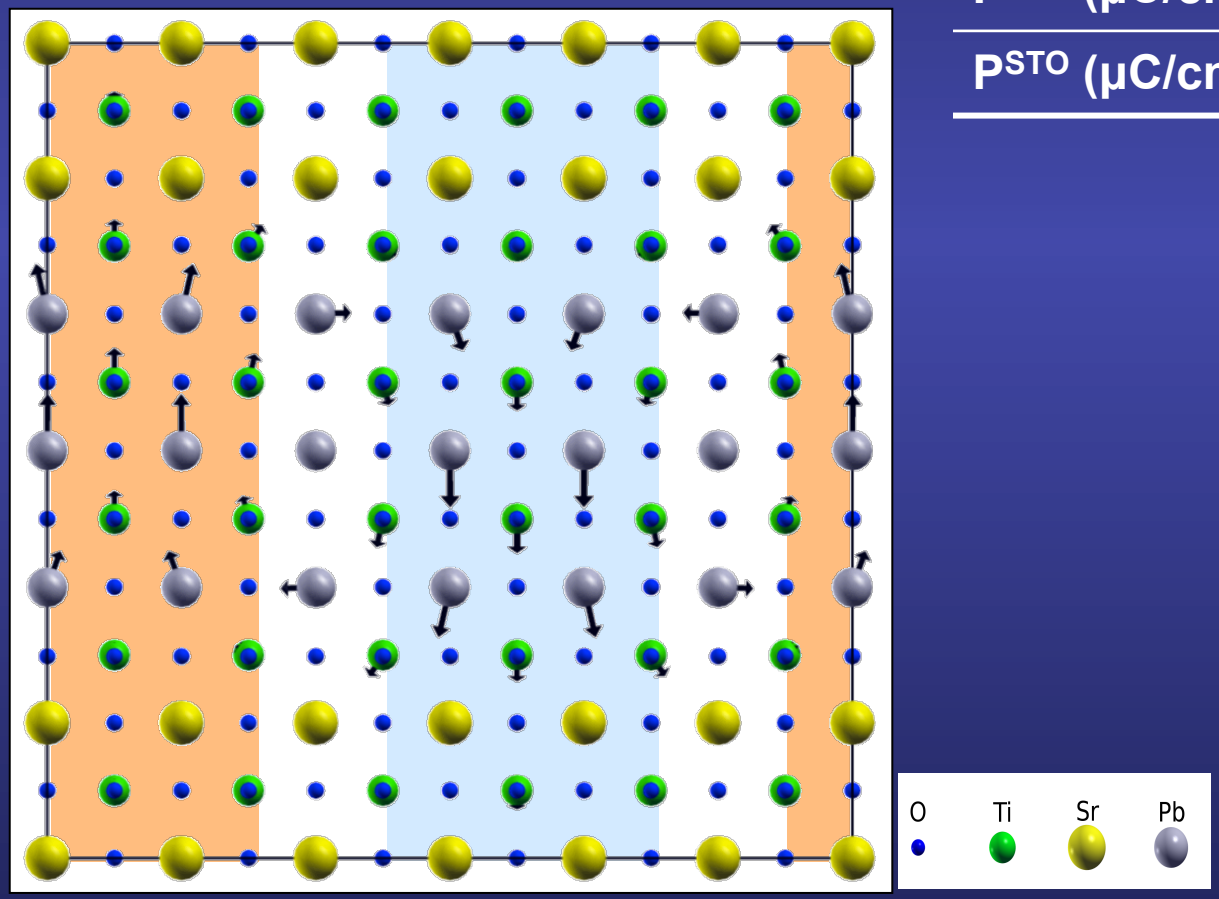


Domains in $PbTiO_3/SrTiO_3$ superlattices: vortices & large polarization

(3,3) superlattice

6 unit cells of domain periodicity

Fully relaxed



Vortices at DW

Polarization domains → good screening

	w/o AFD	with AFD
P^{PTO} (μC/cm²)	(0, 0, 68)	
P^{STO} (μC/cm²)	(0, 0, 25)	

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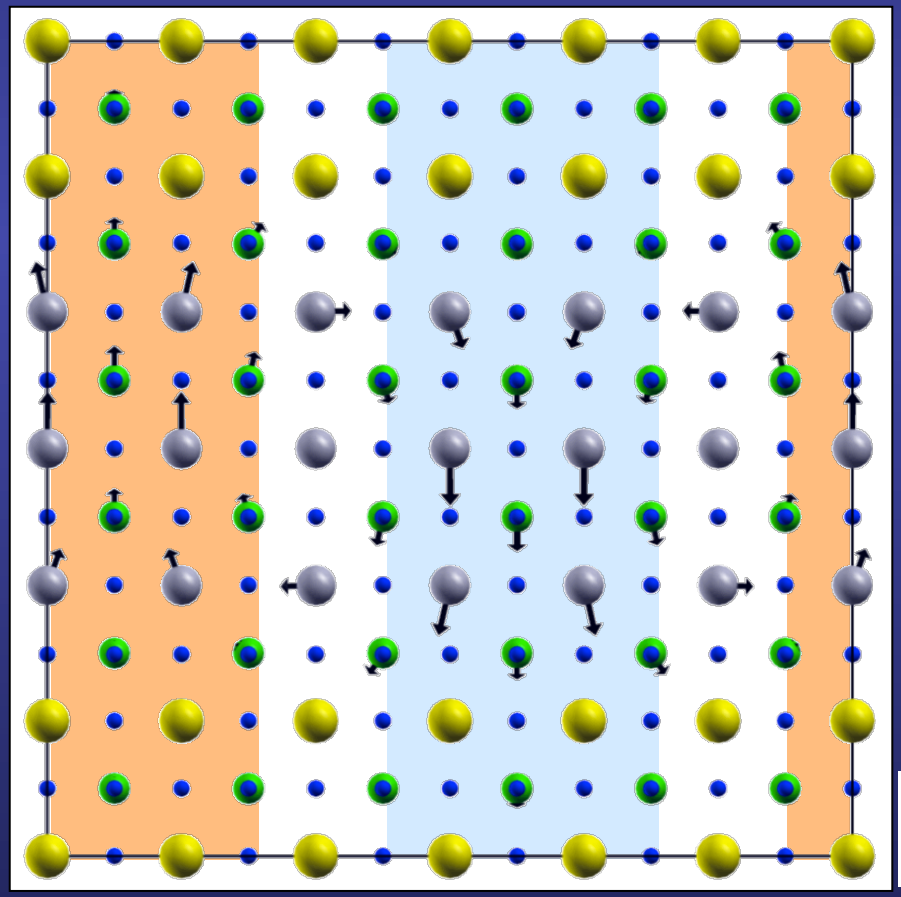

Vortices at DW

Polarization domains → good screening

	w/o AFD	with AFD
P^{PTO} (μC/cm²)	(0, 0, 68)	(0,26,56)
P^{STO} (μC/cm²)	(0, 0, 25)	(0,1,23)