Phonon Related Phenomena in Materials

Umesh V. Waghmare
Theoretical Sciences Unit
also at Centre for Computational Materials Science
Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore 560 064
http://www.jncasr.ac.in/waghmare
http://www.jncasr.ac.in/ccms
waghmare_AT_jncasr.ac.in

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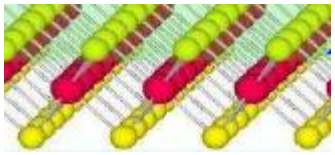
Why Phonons?

- *Fingerprint of a material: Raman, IR spectra*
- Thermodynamic stability: vibrational entropy T, soft modes
- Properties: elastic, dielectric, piezoelectric, etc (couple with fields)
- *Structural Transitions: instabilities of a structure* $w \rightarrow 0$
- *Phonons coupled with electrons*, spin, exciton, polarons; e.g. superconductivity

Emergence of Ferroelectricity at a Metal-Semiconductor Transition in a *1T* Monolayer of MoS_2



Dipolectronics

Sharmila N Shirodkar, Anjali Singh & UVW

Theoretical Sciences Unit

J Nehru Centre for Advanced Scientific Research, Bangalore 560 064

www.jncasr.ac.in/waghmare

JNCASR

Funding from DST and DAE, Government of India

Collaborators

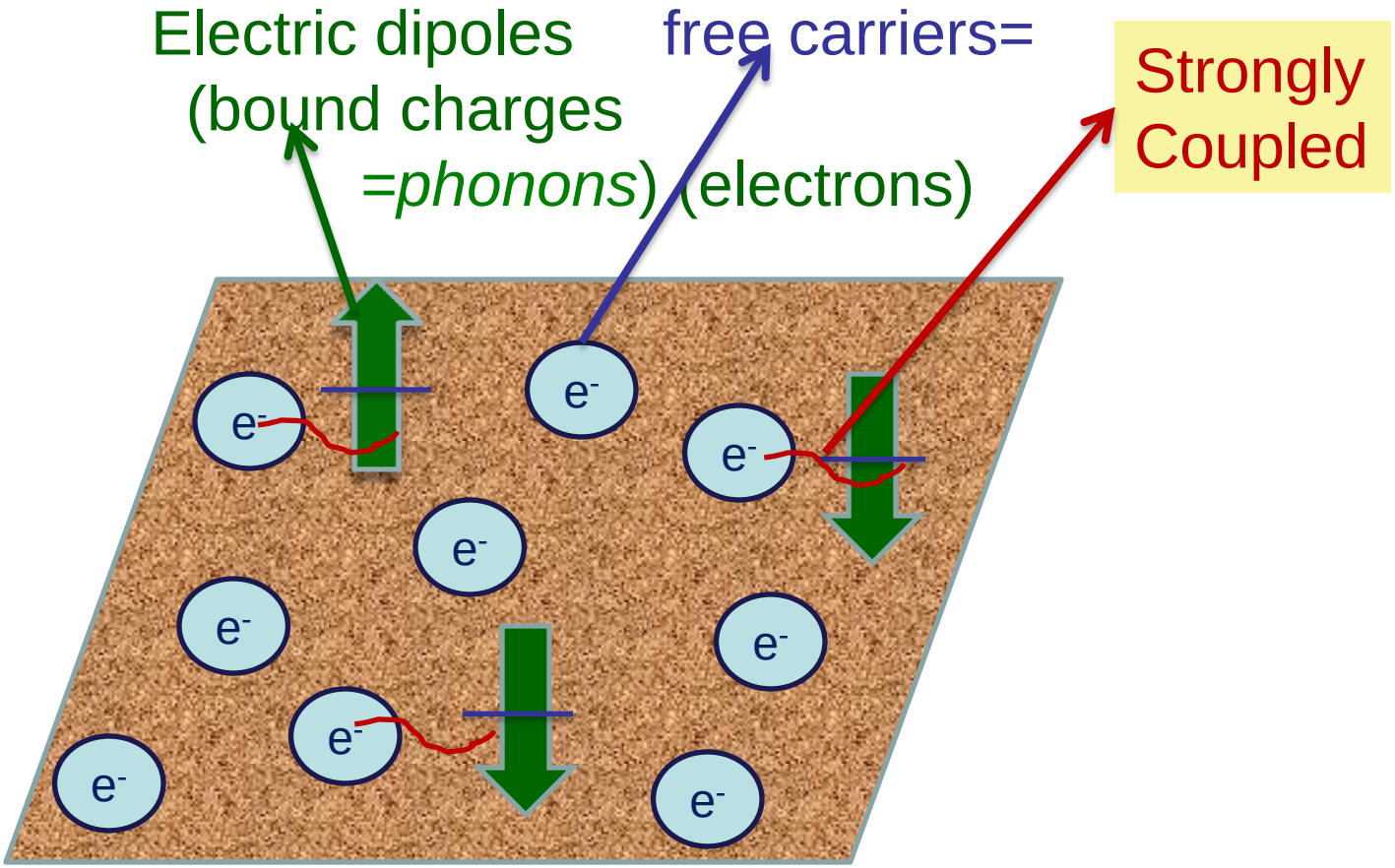
- Sharmila N Shirodkar (JNCASR)
- Anjali Singh (JNCASR)

Experiments and Stimulating Collaborations:

- CNR Rao and Group (JNCASR)
- Ajay K Sood and Group (IISc)

Take-Home Message: *1T* MoS_2

Ferroelectric Semiconductor



(nano)

Propose new class of devices: *Dipolectronics*

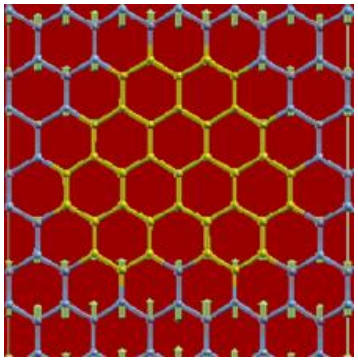
S N Shirodkar and U V Waghmare, Phys Rev Lett. 112, 157601 (2014).

2-D Nano-materials

- Graphene: High mobility, Low on/off ratio
- BN: A good insulator, too low mobility
- $C_x(BN)_{1-x}$: Domains of BN

  vs disorder

  VRH conduction

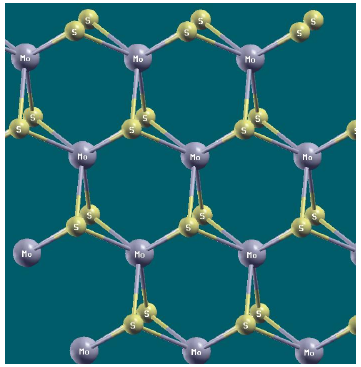


- MoS_2: Intermediate gap, good on/off ratio

Holds promise for nano-electronic applications

Massive Dirac Fermionic nature

Spin split bands

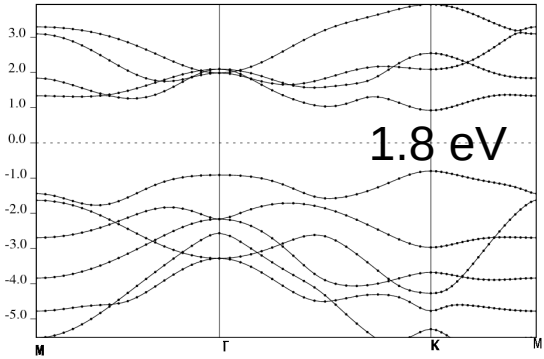


FET: Kis et al, Nature Nano 6, 107601 (2011)

FET based Sensors:

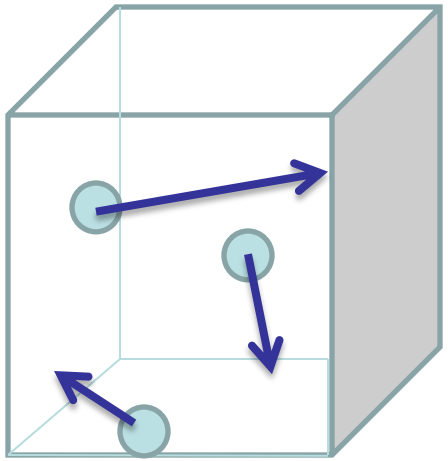
Rao, Dravid, UVW et al ACS Nano (2013)

Frontier: Rao, Maitra and UVW, CPL (2014)

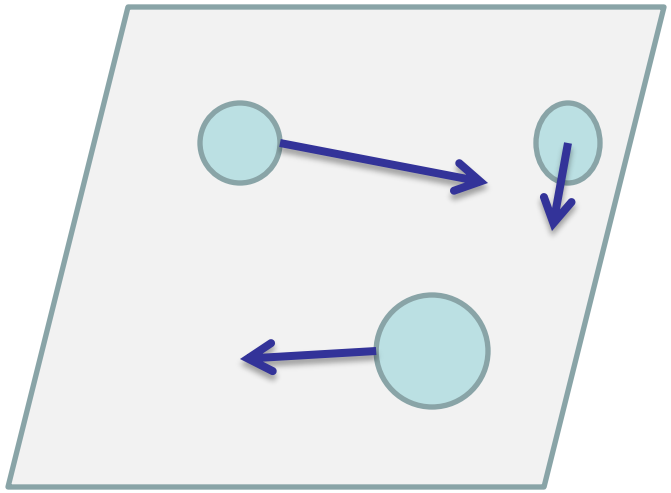


Electron-phonon Coupling

Low Dimensionality:



3-D
Low probability

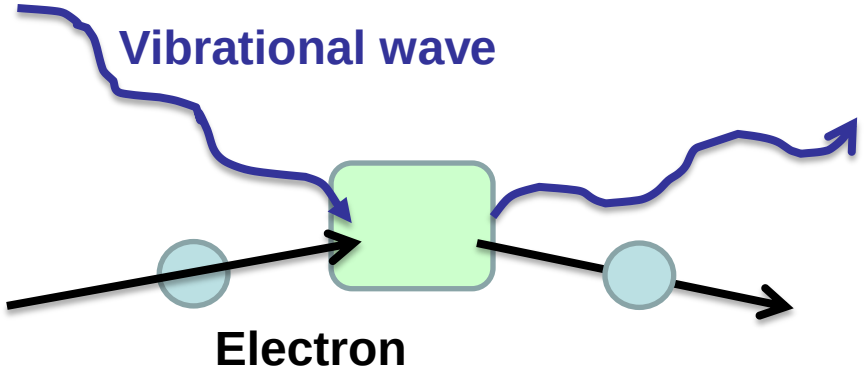


2D
High probability to collide

- Coupling between degrees of freedom is more readily possible
- Such coupling can have more drastic consequences
- Sensitivity to external Fields:

  As long as the symmetry allows it!

Electron-phonon Coupling



Examples in Low-dimensional Systems

Bredas et al, Acc Chem Res 18, 305 (1985)

Polarons:
Conducting Polymers

www.nobelprize.org

Z X Shen et al, Phys Rev Lett 110, 265502 (2013).

Quasi-1D cuprates: "Our results indicate that the lattice degrees of freedom are fully integrated into the electronic behavior in low-dimensional systems."

Electron-Phonon Coupling (EPC) in Graphene

EPC results in changes in phonon frequencies with doping:

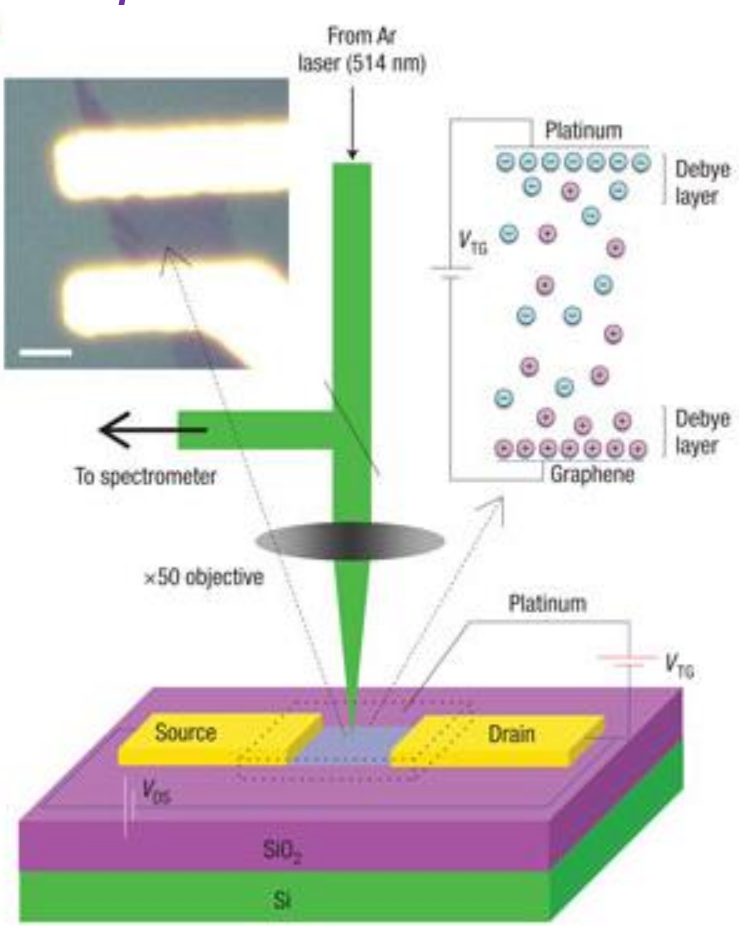
key to use of Raman for characterization of devices

Sood et al, Nat Nanotech. (2008).

Electric Field Effect Tuning of EPC in graphene:

Gate voltage changes *w* of G-band

Pinczuk et al, Phys Rev Lett. (2008).

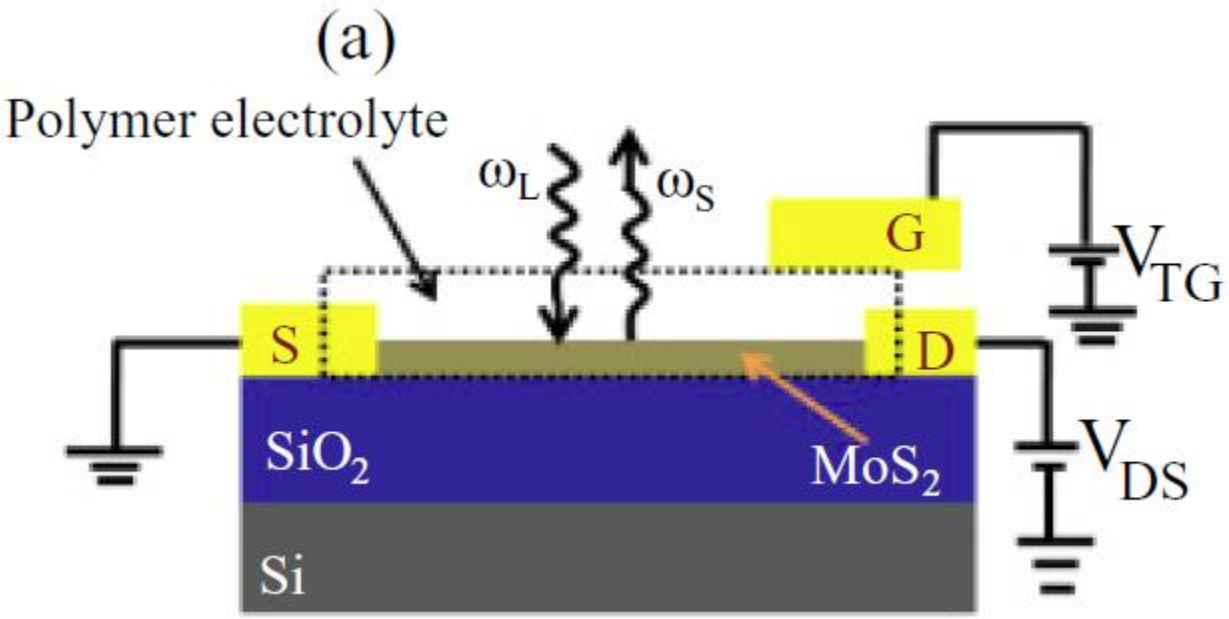


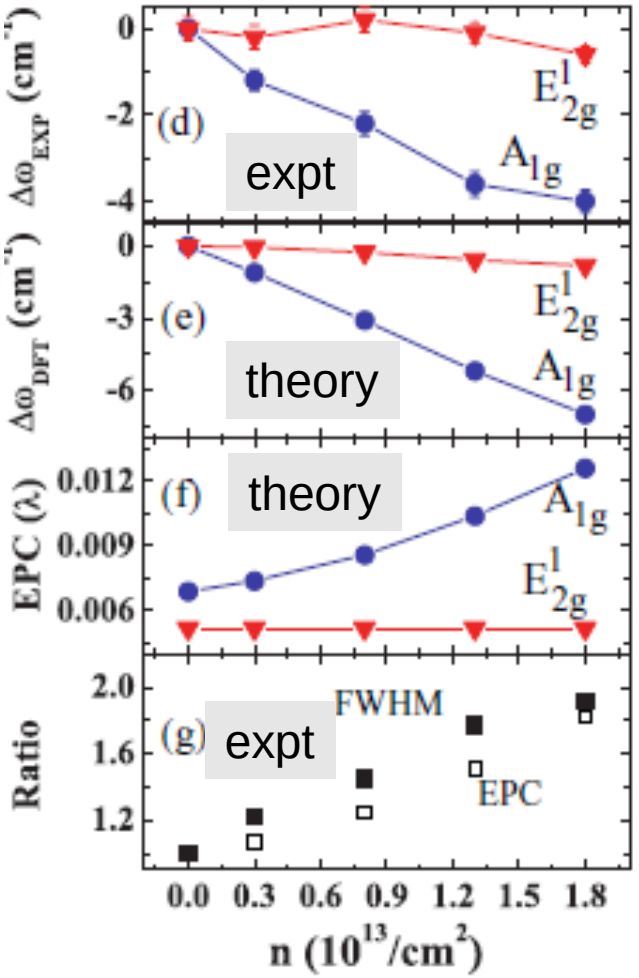
Breakdown of Born-Oppenheimer Approximation!

Motion of e and phonon *can not* be decoupled

Pisana et al, Nat Mat. (2007).

Electron-Phonon Coupling (EPC) in MoS_2





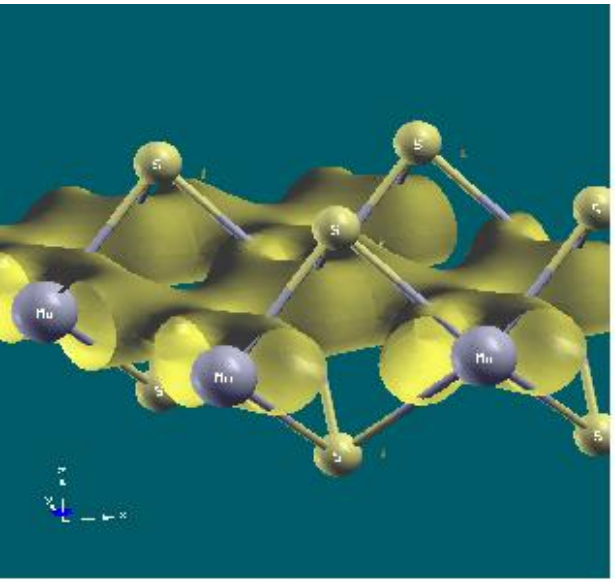
Gate field: change doping level

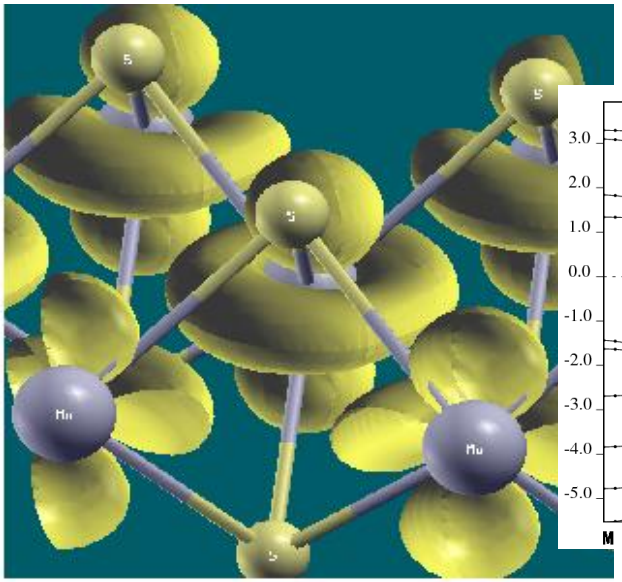
It affects specifically A_{1g} mode. Theory reproduces both w and relative changes in line-width

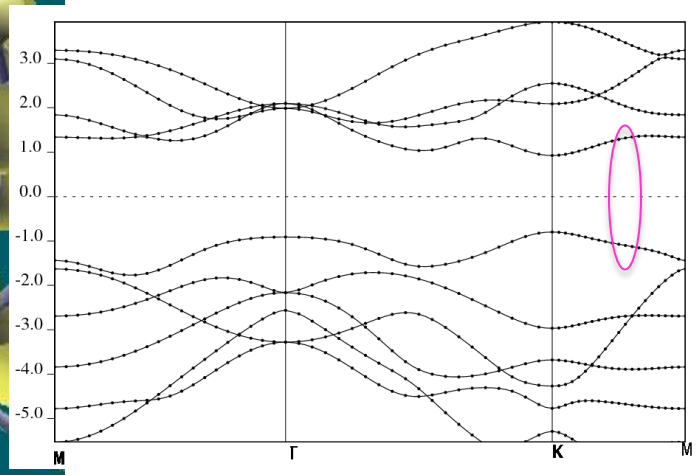
Chakraborty, Bera, Muthu, Bhowmick, Waghmare and Sood, Phys Rev B 85, *R* 161403 (2012) Editor's Suggestion.

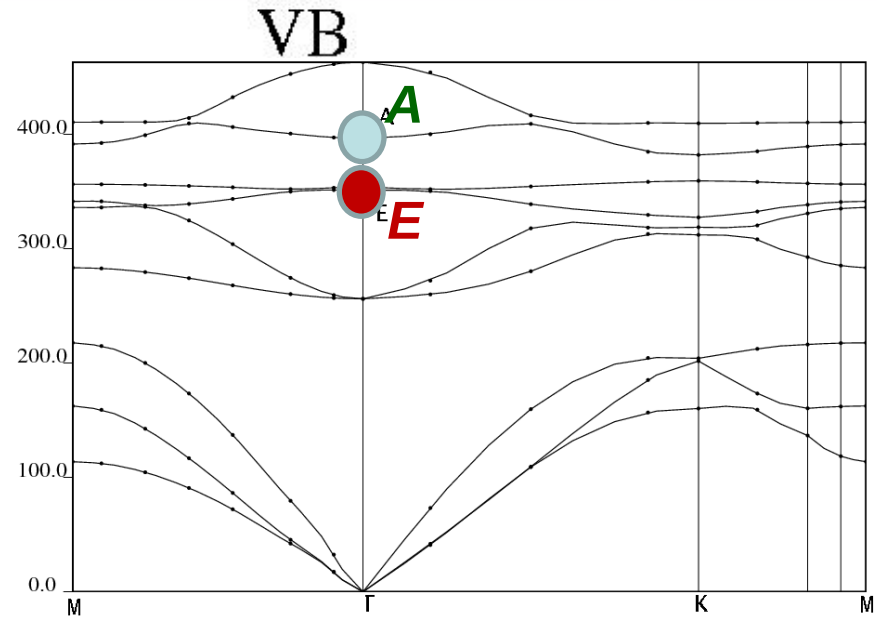
Large Coupling of A_{1g} Mode with Electrons

States on the two sides of band gap at K-point









CB Sood et al, Phys Rev B 85, *R* 161403 (12

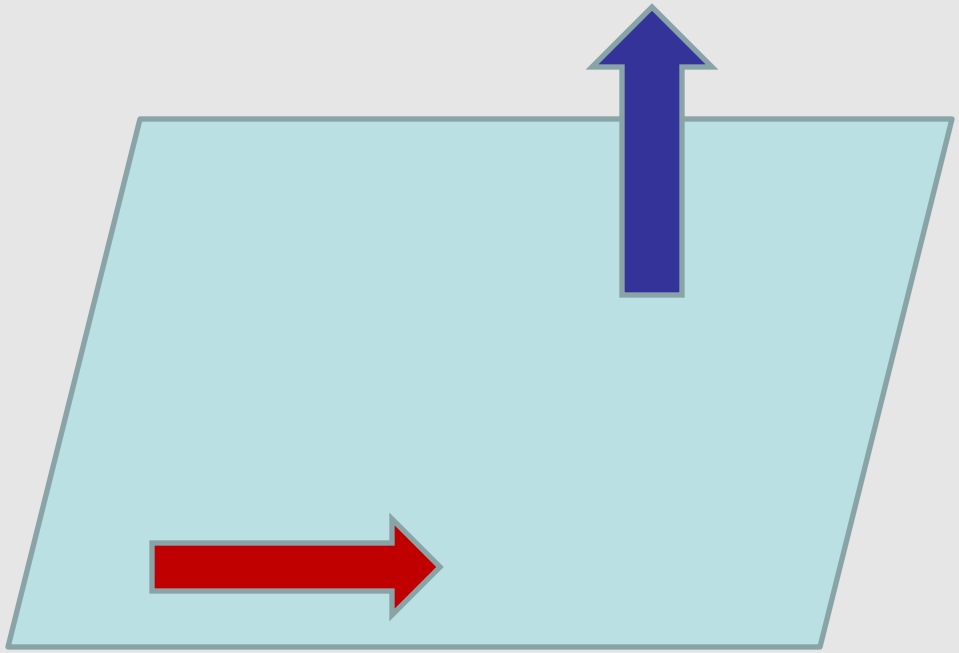
CB: Full symmetry of the system (A_{1g} representation)

only $\langle A_{1g} | \Delta V(A_{1g}) | A_{1g} \rangle \neq 0$!

Symmetry dependent phonon renormalization

Raman: Characterization of FET

So far, effect of $\perp$ *electric field* on 2-D materials has been investigated.



What if the field is *in-plane*?

→ Metallic 2-D materials *will just conduct!*

→ Semiconducting ones may do something interesting!

Tunability of Electron-phonon Coupling with *In-plane* Electric Field

→ Electro-resistance, polarons

A generic property of the 2-D materials

Tuning EPC with Electric Field

Electron-phonon coupling matrix element

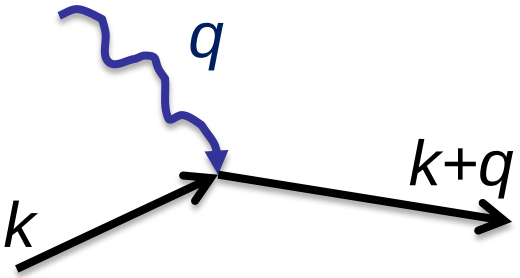
$$\lambda_{q\nu} = \frac{2}{\hbar\omega_{q\nu}N(\epsilon_f)}\sum_k\sum_{mn}\left|g^{q\nu,ij}_{k+q,k}\right|^2 \times \delta(\epsilon_{k+q,i}-\epsilon_f) \times \delta(\epsilon_{k,j}-\epsilon_f), \quad (1)$$

Density of States

$E_\perp$ changes doping, ε_F, the occupation numbers: *DoS*

We show that the *in-plane E* changes the matrix element *(for q=0)*:

$$g^{q\nu,ij}_{k+q,k} = \left(\frac{\hbar}{2M\omega_{q\nu}}\right)^{\frac{1}{2}} \langle\psi_{k+q,i}|\Delta V_{q\nu}|\psi_{k,j}\rangle,$$



Expand series in E

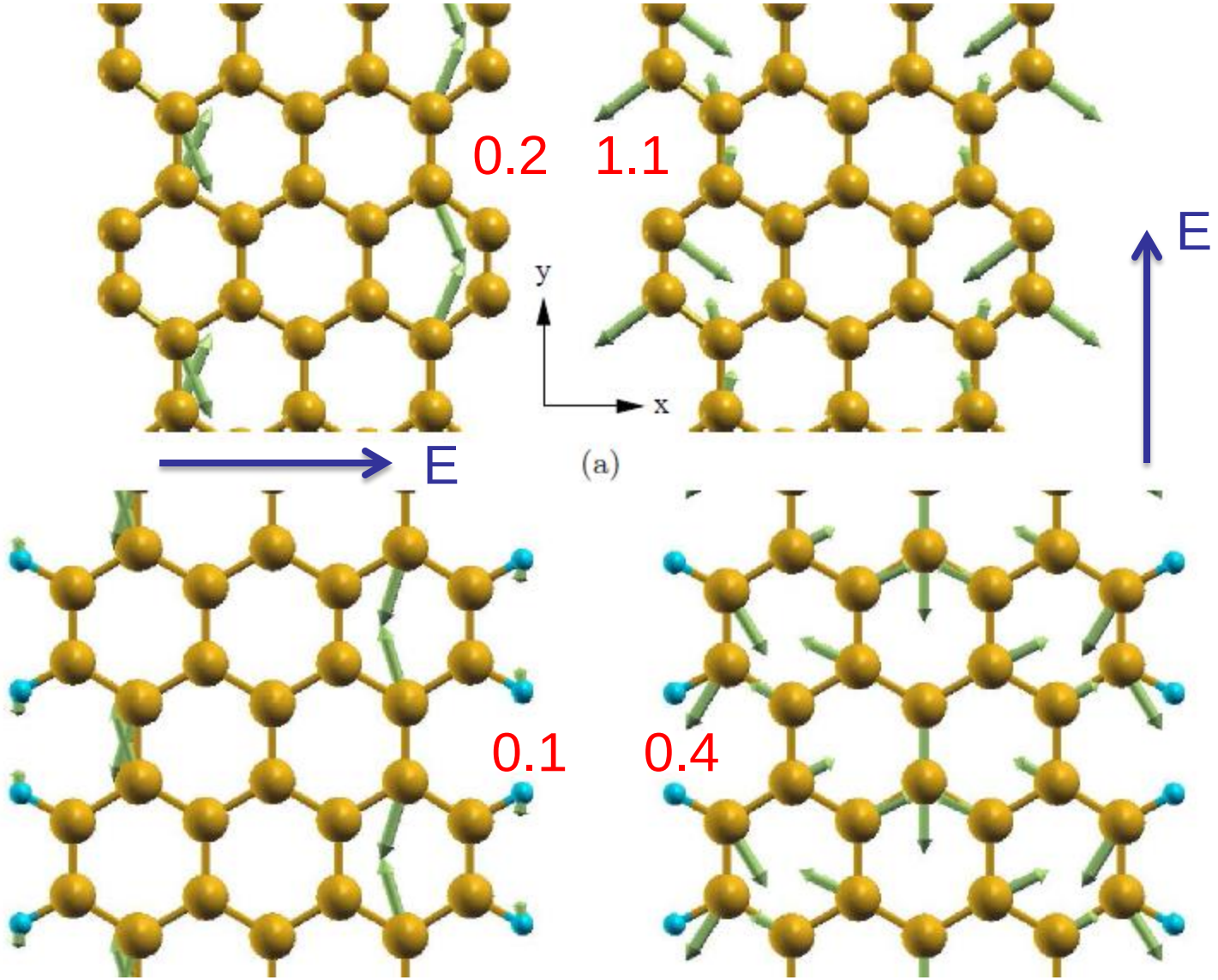
$$\langle k,m\sigma|\nabla_{\mathbf{R}_n}V_{el-i}|k,n\sigma\rangle + EZ_{n,\alpha,\beta}(k,n)\delta_{m,n}$$

Force

Tunability Parameter

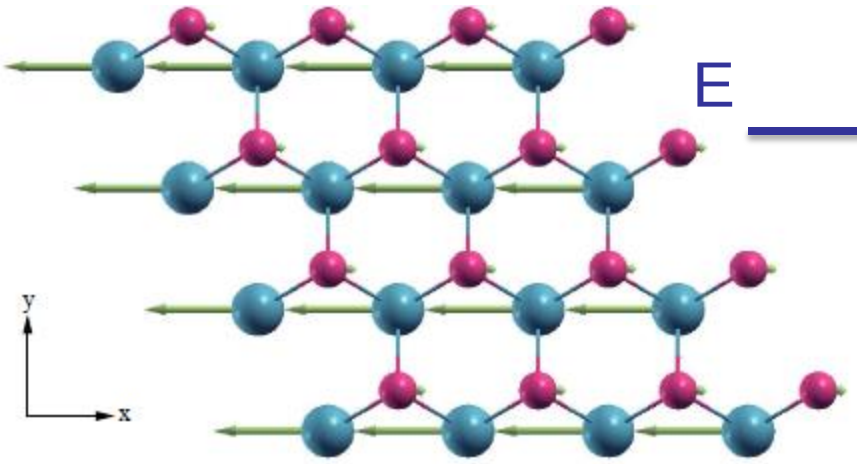
CHARGE: Force on an atom by E

Graphene Nano-ribbons

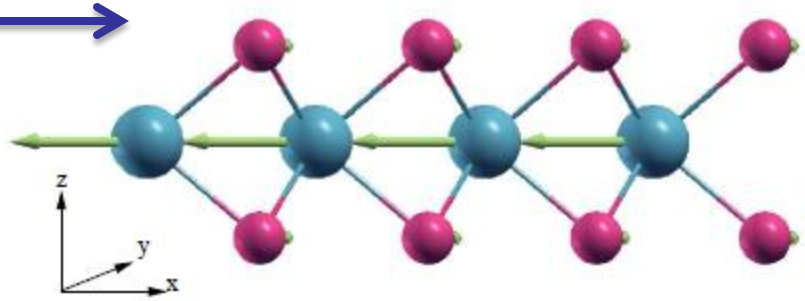


States localized on edges, force felt by the ions there!

EPC(E): Dynamical Charges in MoS_2



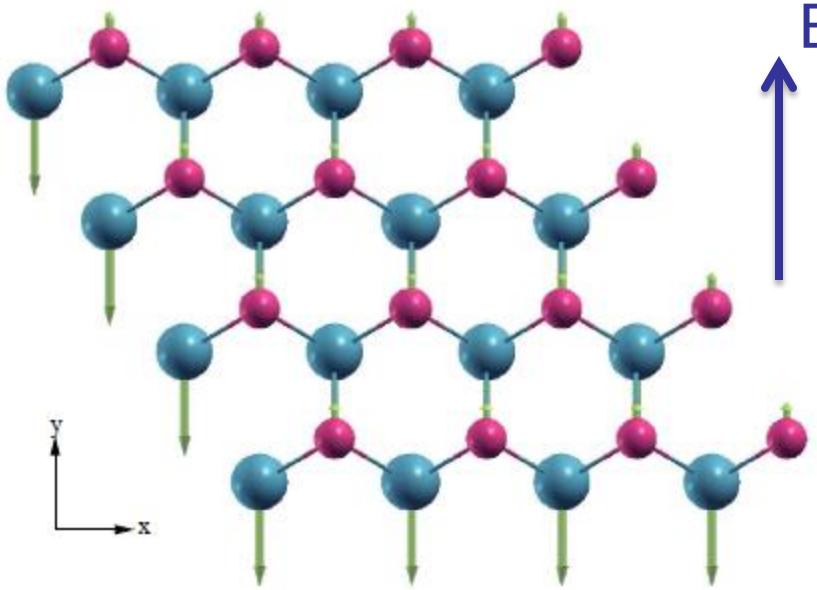
E

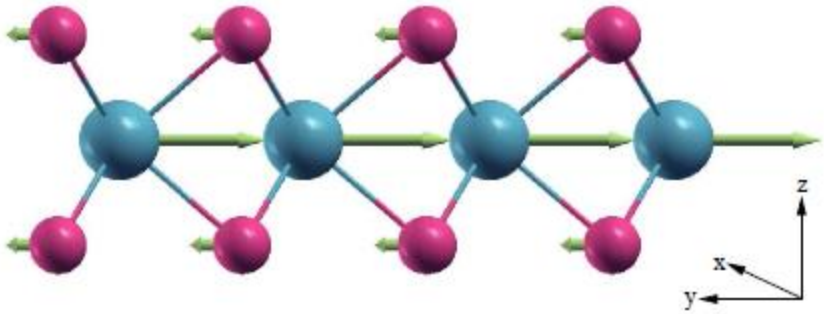


	MoS_2	TiS_2
Z(Mo)=-1.14	Z(Ti)= 8.8 x	
-0.91	8.8 y	

(a)

E





Anomaly: even the sign of charge is counter-intuitive!

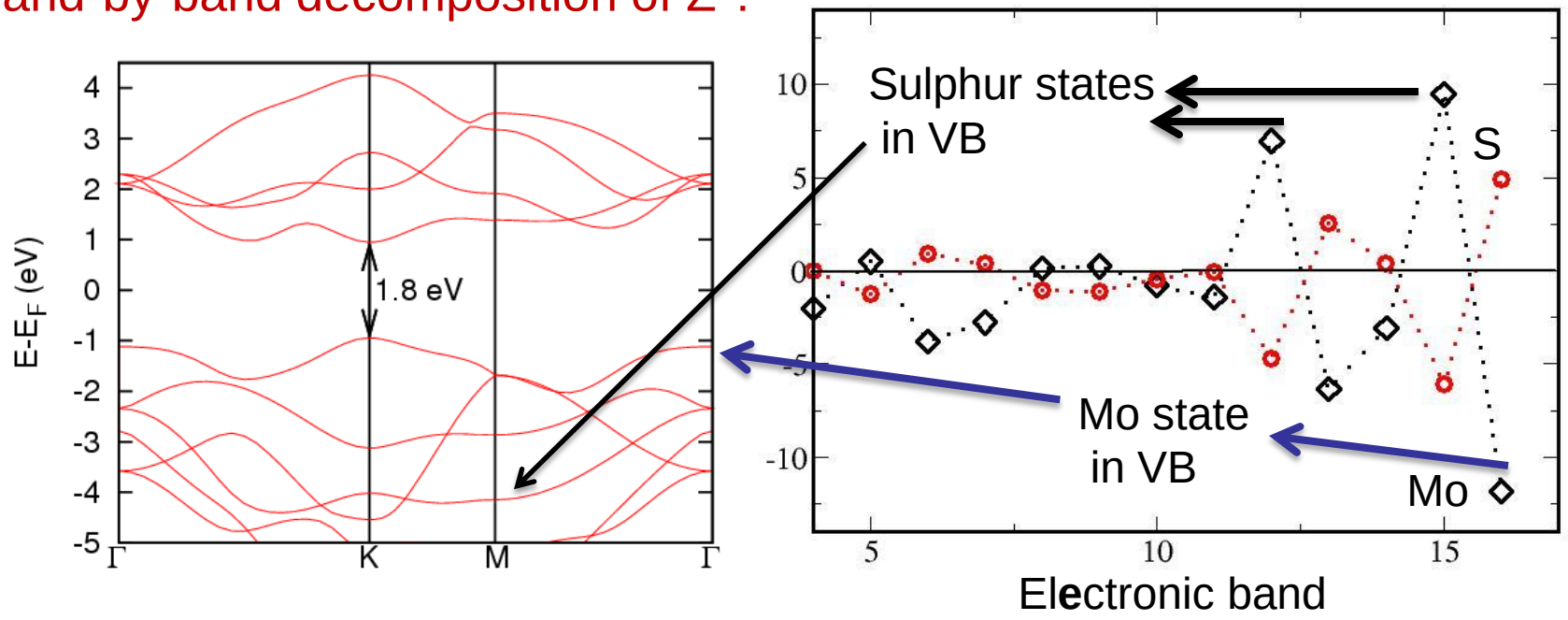
Tunability of EPC (MoS_2) with in-plane electric field

Anomalous dynamical charges:

Z*(Mo)= -0.8 to -1.0, depending on the method used

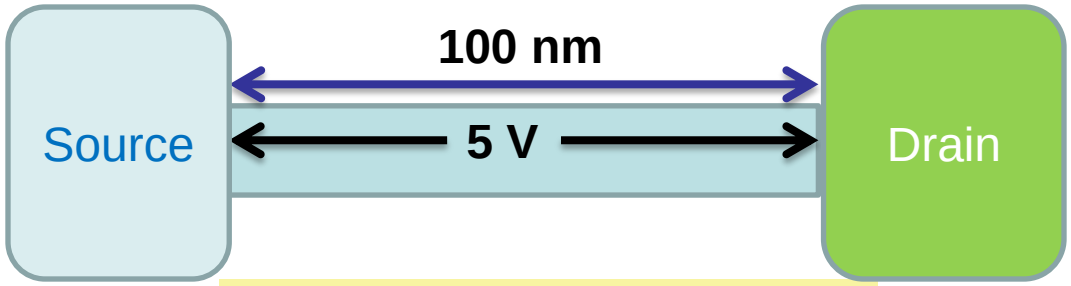
Z* (S) = 0.4 to 0.5!

Band-by-band decomposition of Z*:



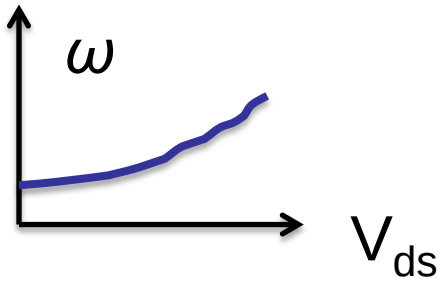
Coupling of top of the valence and bottom of the conduction *e* states with *Phonons* most tunable with electric field!

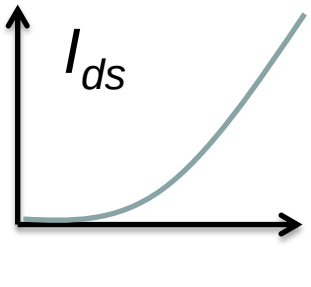
Predictions for experiments (MoS_2)



For a field *E = 500 kV/cm*,
Electron phonon coupling
to change by > 10 %

→ *IR/Raman* → *Electro-resistance*





Nonlinearity

So far, we find in *2H* MoS_2:

- Strong electron phonon coupling (EPC)
- Strong dependence of EPC on electric field
- Highly anomalous dynamical charges

Waghmare, Kandpal, Spaldin and Seshadri, PRB (2003).

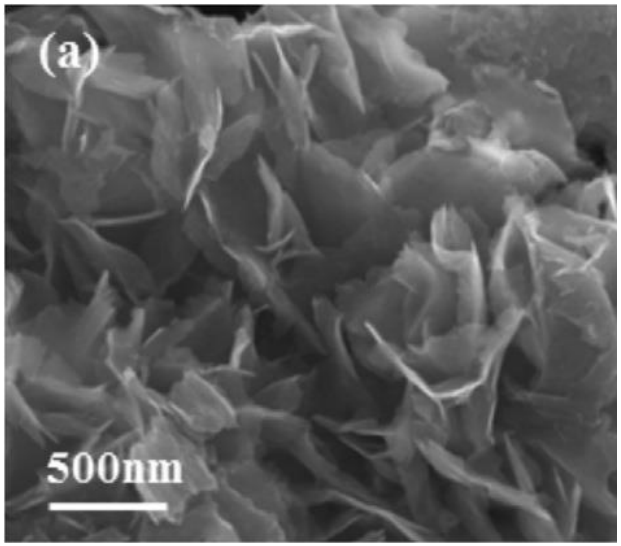
► *Tendency of a material to turn metallic*
► *Tendency to be ferroelectric*

The usual *2H* form of MoS_2:
not a good candidate (is non-centrosymmetric, but P=0, because of other symmetries)

►Is there a metallic state in *the* structural neighborhood?

Prof. Rao's experiments gave us a hint!

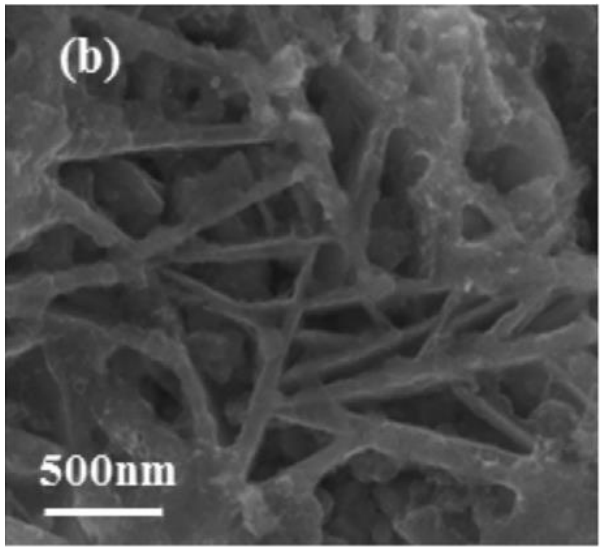
Ironing out MoS_2 or $MoSe_2$

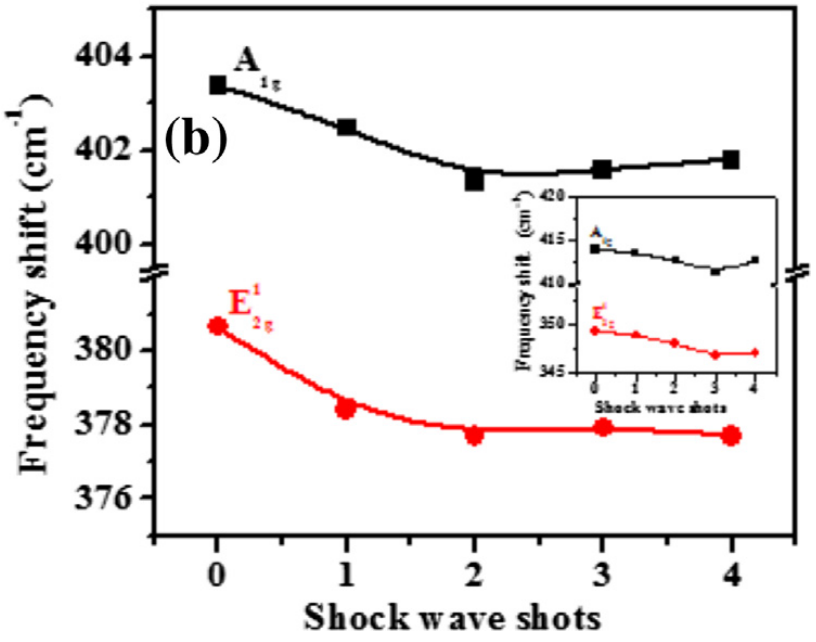


$MoSe_2$

High T
Shock Waves

Reduction in d
(interplaner spacing)





CNR Rao et al, Chem Phys Lett 582, 105 (2013)

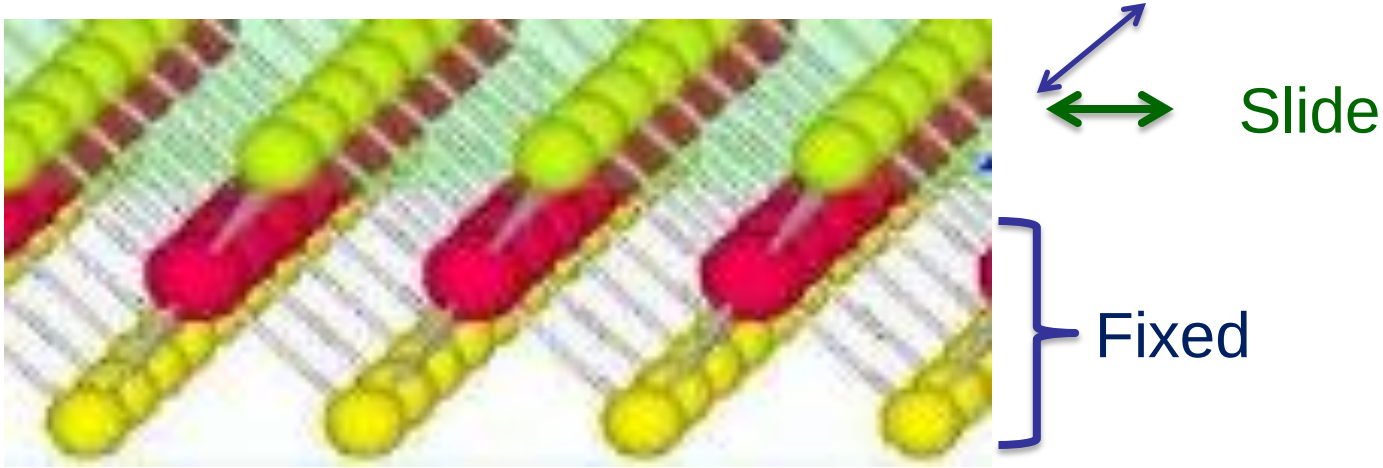
Two-stage mechanism:

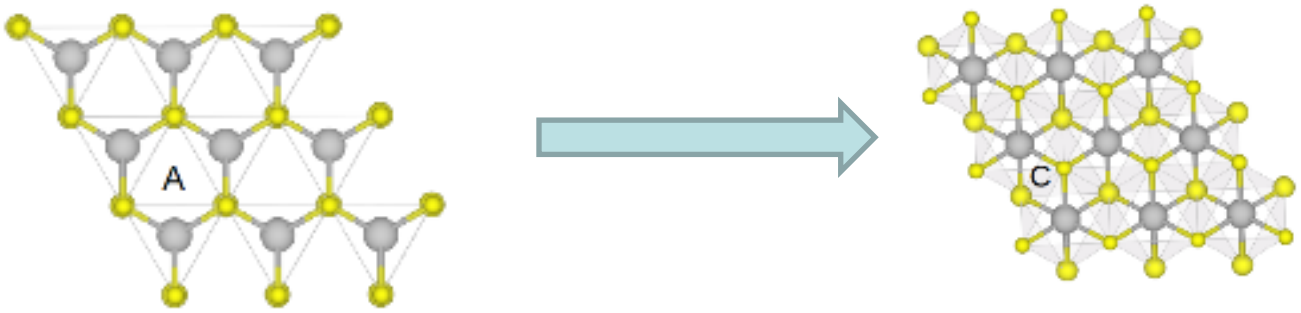
(i) Flattening of sheets through shear+uniaxial strains

(ii) Mainly compression along c-axis

SHEAR STRAIN within a Monolayer

Shearing MX_2 sheets



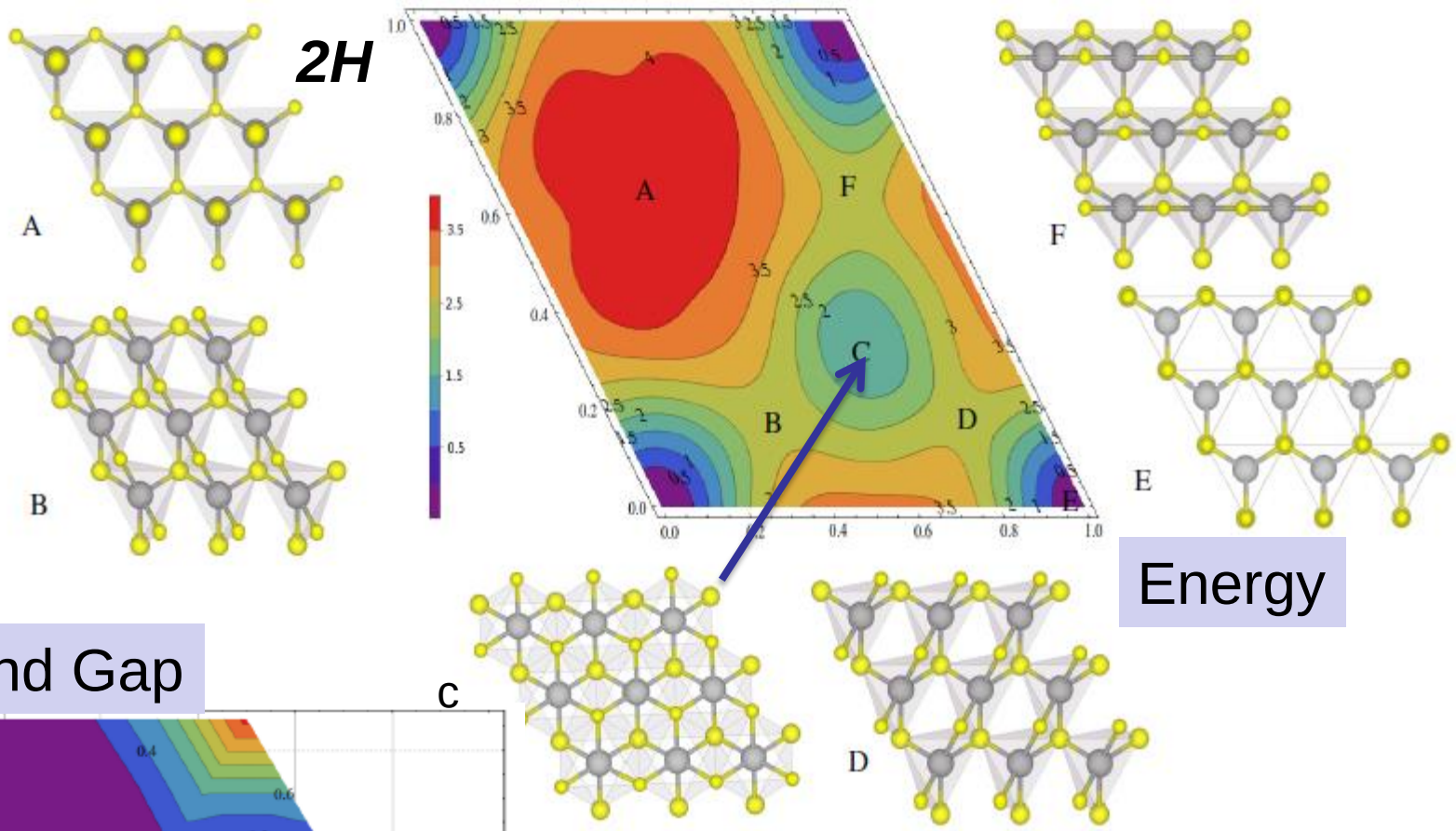


2H ***1T***

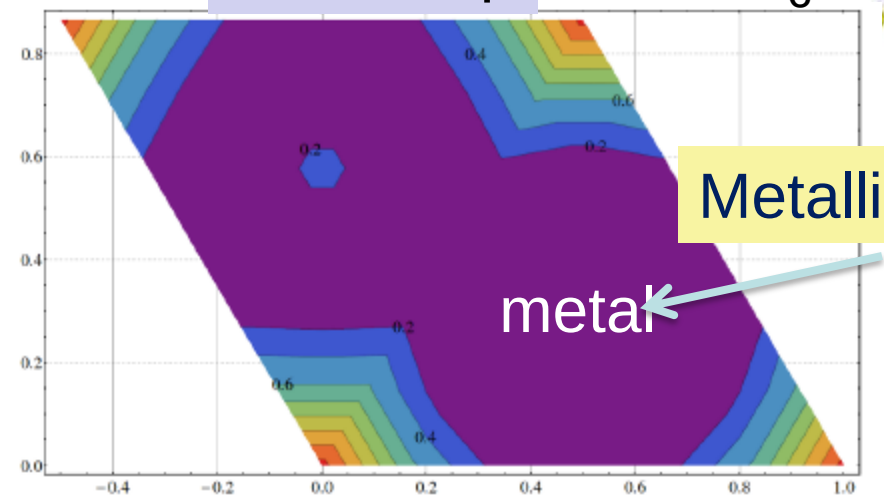
What is the energetics?
How does the band-gap change?

MoS_2 *monolayer:*

Generalized shear strain *(SLIP)* response



Band Gap

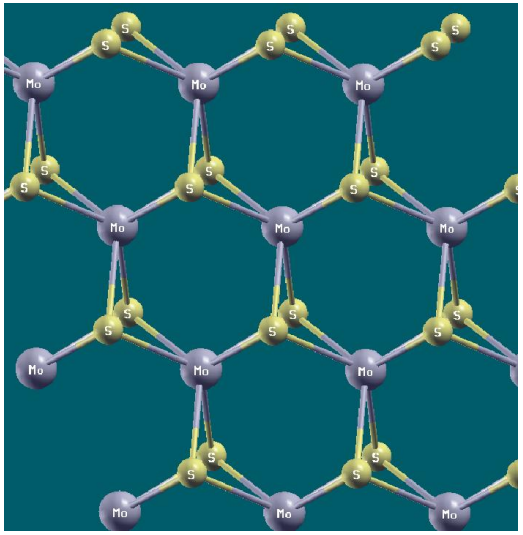


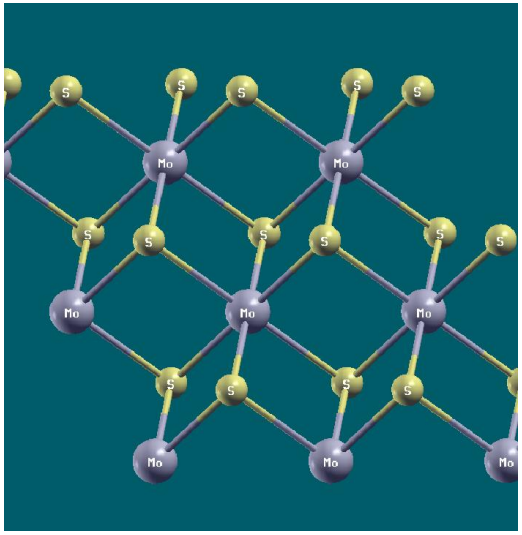
Metallic *1T* polytype

A Singh, Shirodkar and Waghmare (preprint)

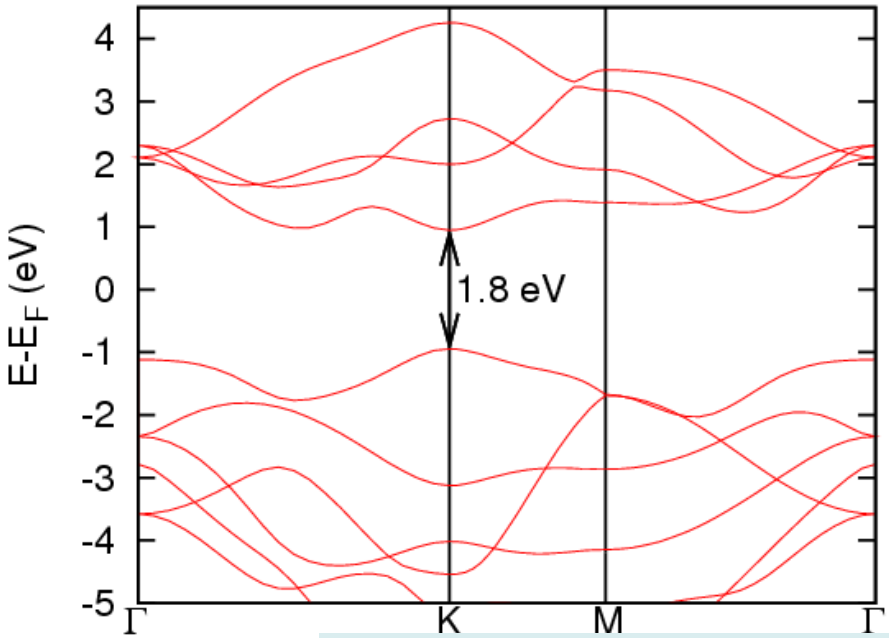
MoS_2: Insulator

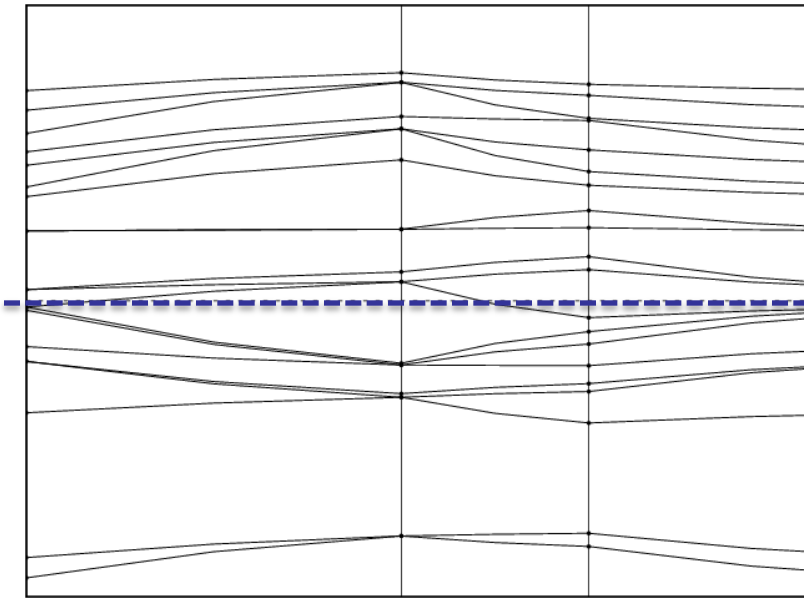
Metal





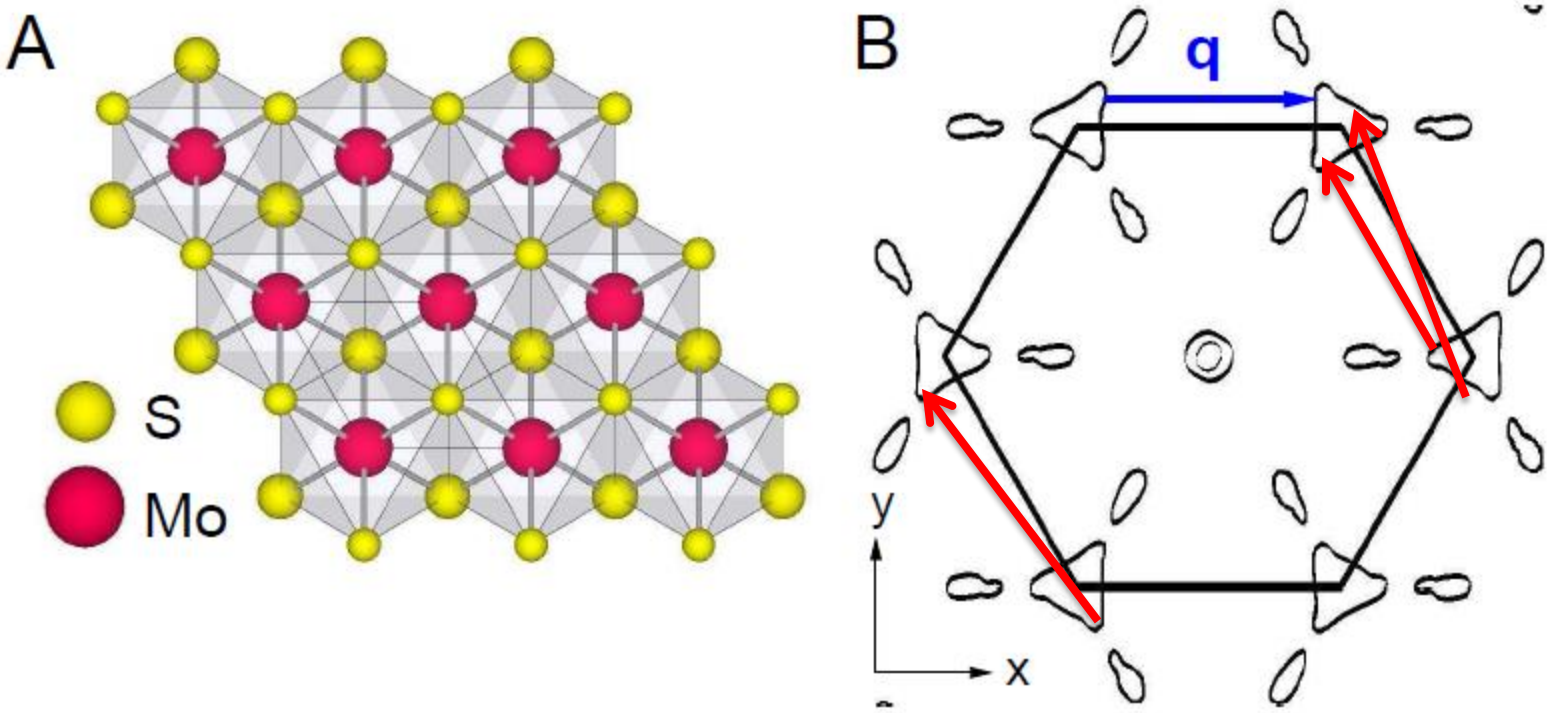
2H *1T*





Resemblance to Bi_2Te_3: a topological insulator

Structure of the *1T* Polymorph of MoS_2



- Structure is *Centro-symmetric*
- Fermi surface is *weakly nested* by q-vectors that form an equilateral triangle centred at *K*

"Average nesting" by *K: instability*

Charge Density Wave
Lattice Wave: Phonon

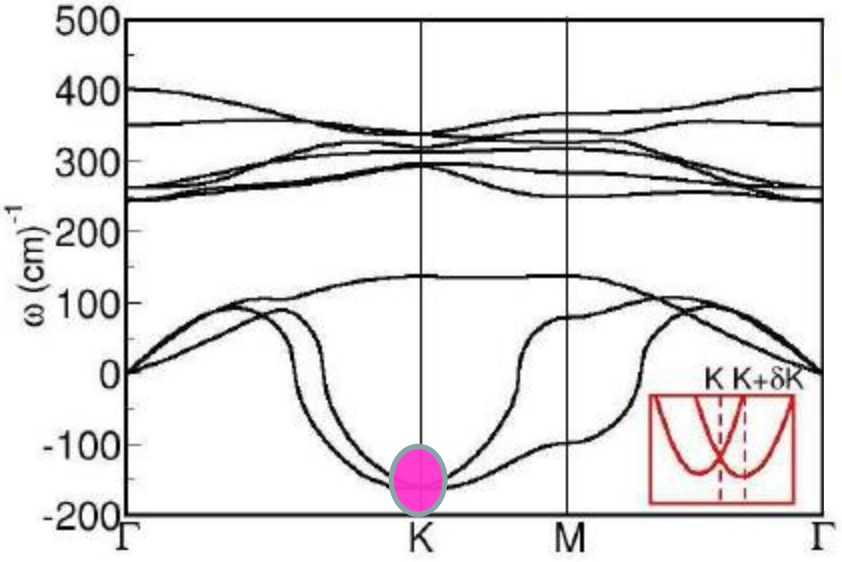
Fermi Surface Nesting:

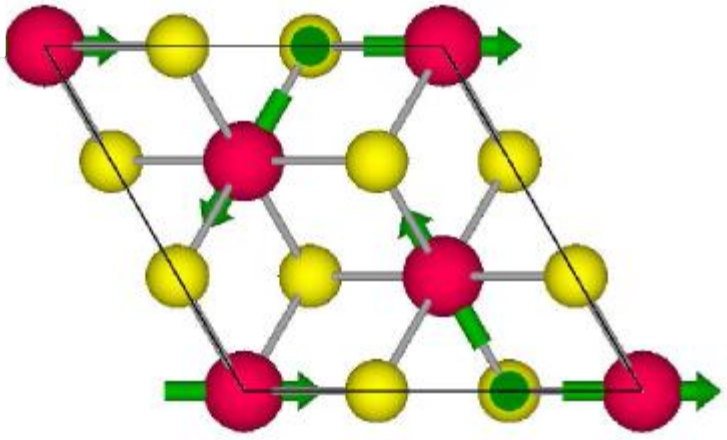
Many electronic states on the Fermi-surface can be scattered by a phonon with nesting wave vector to other states on the Fermi-surface

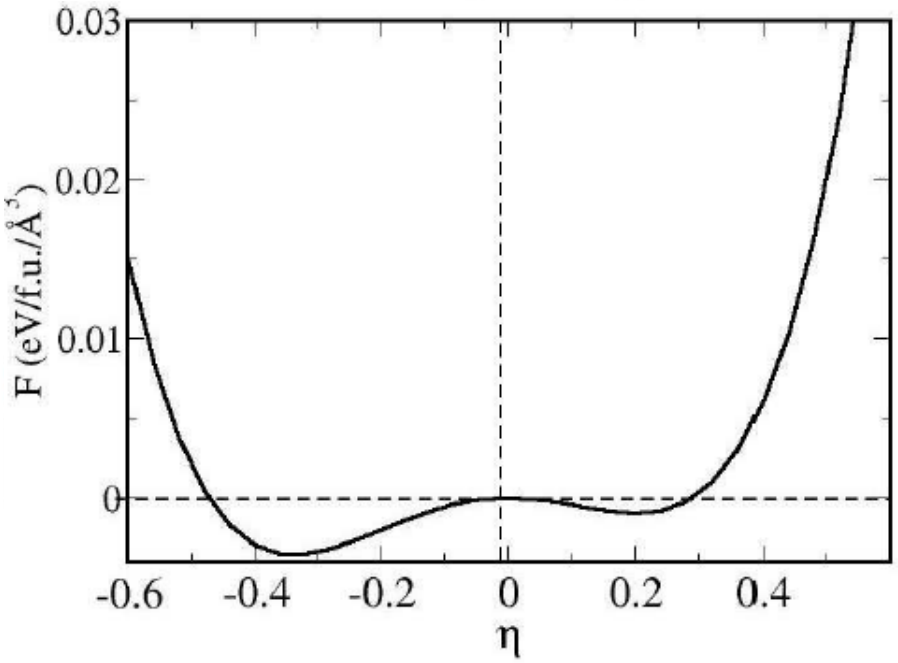
Structure is unstable:

Perturbation with that phonon drives the structure *to lower energy!*

Cell-tripling Structural Instability





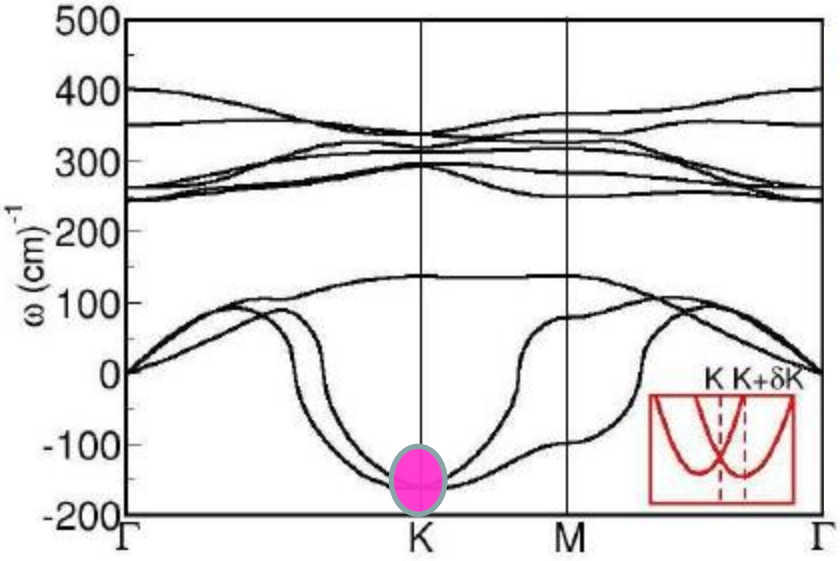


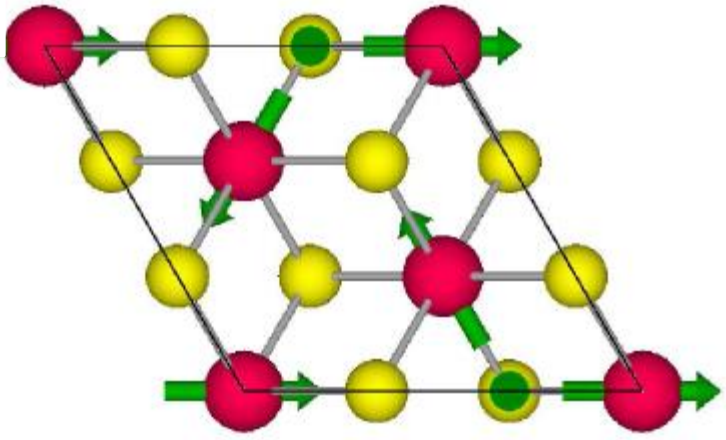
Strongest instability at *K:*

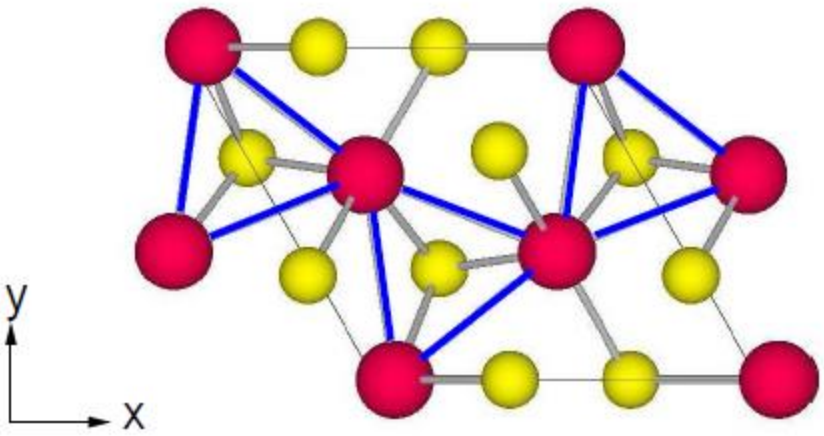
distortion of the structure leads to lower energy "stable" structure

Mo-trimerization

Cell-tripling Structural Instability



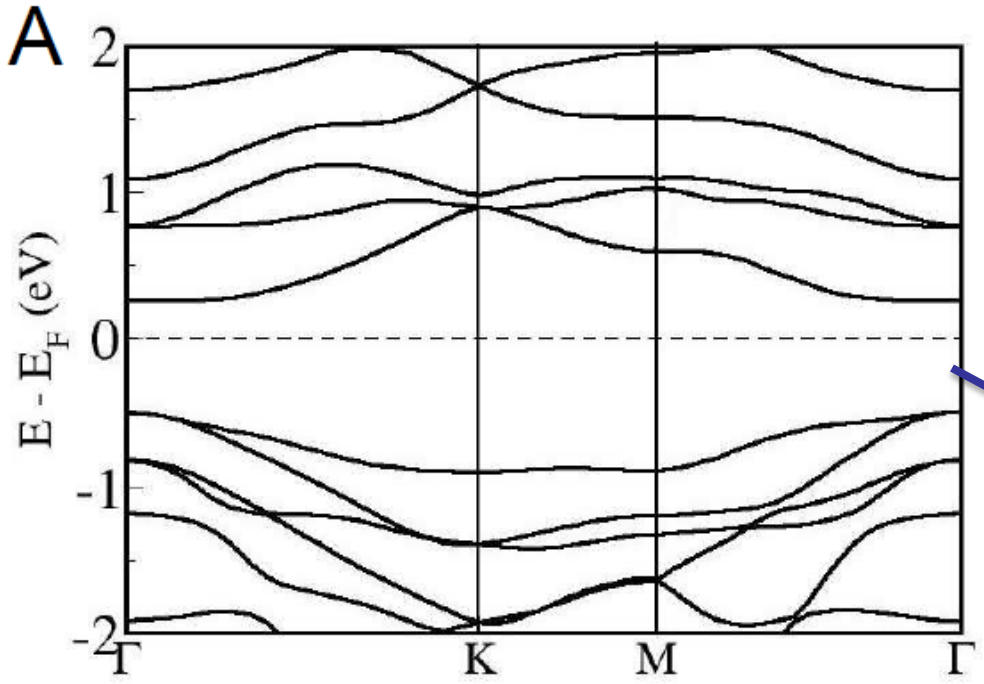




Strongest instability at *K*

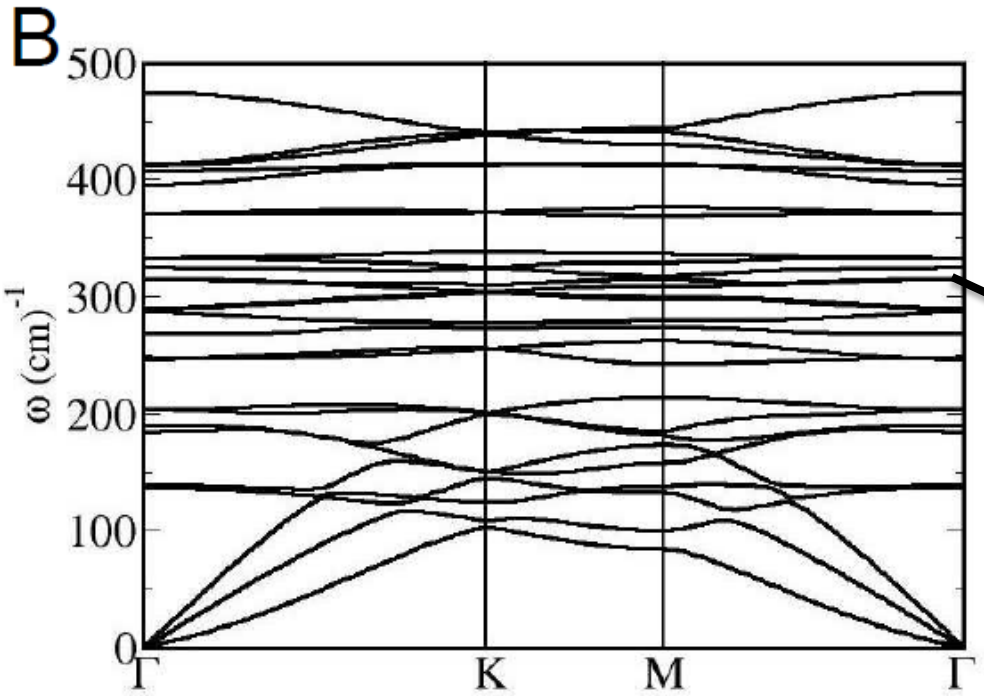
Leads to Mo-trimerization

What happens to Electronic Structure?



Mo-trimerized structure (*d1T*):

1. *Semiconducting*
   E_g=0.7 eV

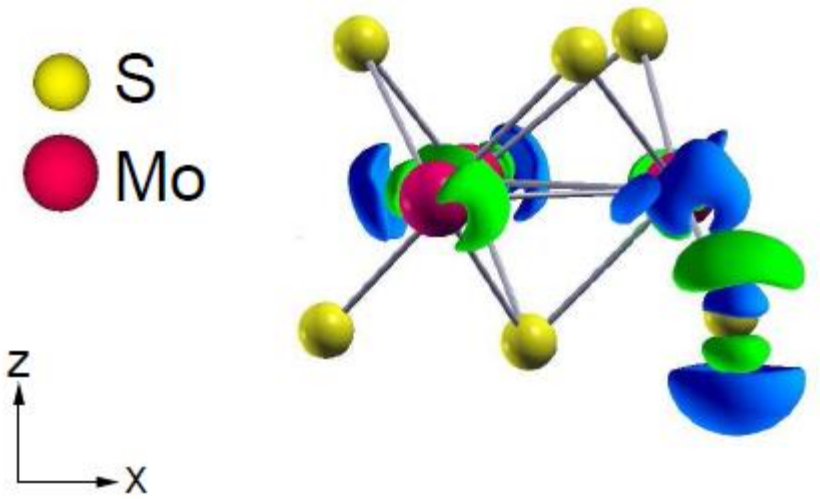


2. *Locally stable:*
   phonon dispersion
   Raman Sign A_{1g} mode at 321 cm^{-1}

What happens to inversion symmetry?

Broken inversion symmetry: Difference density

d1T-c1T



K: zone boundary point
periodic modulation

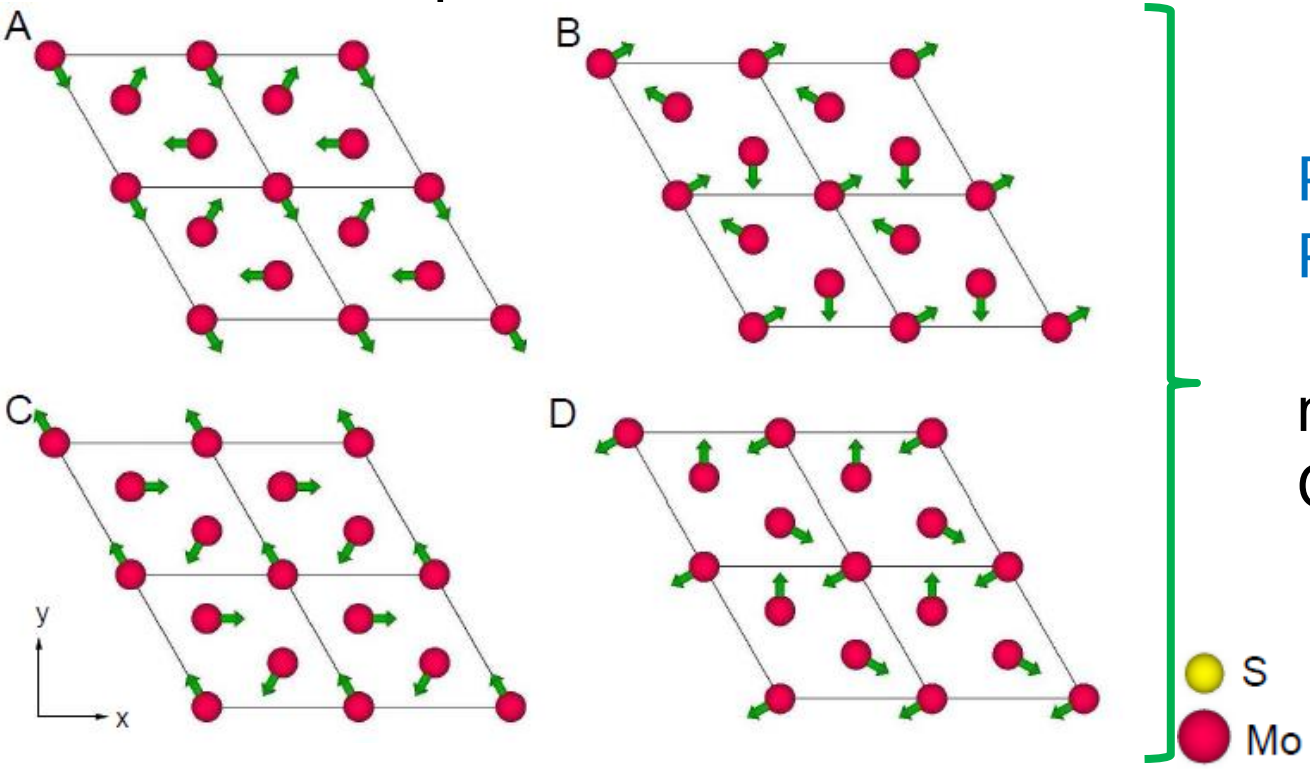
Can *not* give a uniform polarization

Berry phase calculation:
P=0.28 μC/cm^2

Puzzle: Where does the polarization come from?

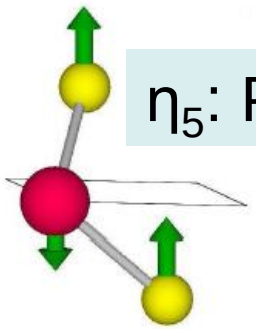
Symmetry Analysis: Landau Theory

Order Parameters: Symmetry invariant subspace of atomic displacements that connect *c1T* structure to *d1T*

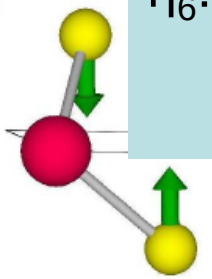


Primary Order Parameters:

η_1, η_2, η_3, η_4
Give *trimerization* of Mo



η_5: Polarization



η_6: "Thickness change" full symmetry

Secondary Order Parameters

Landau Theory: Free Energy of Structural Distortions

$$
\begin{aligned}
F = {} & g_{12}\,(\eta_1^2+\eta_2^2+\eta_3^2+\eta_4^2) + g_{22}\,\eta_5^2 \\
& + g_{13}\,(\eta_1^3 - 3\,\eta_1\,\eta_2^2 + \eta_3^3 - 3\,\eta_3\,\eta_4^2) + g_{23}\,\eta_5(\eta_1^2+\eta_2^2-\eta_3^2-\eta_4^2) \\
& + g_{14}\,[(\eta_1^2+\eta_2^2)^2 + (\eta_2^2+\eta_3^2)^2 + (\eta_3^2+\eta_4^2)^2 + (\eta_4^2+\eta_1^2)^2 + (\eta_3^2+\eta_1^2)^2 + (\eta_4^2+\eta_2^2)^2 \\
& \quad - 2\eta_1^4 - 2\eta_2^4 - 2\eta_3^4 - 2\eta_4^4] \\
& + g_{24}\,[(\eta_1^2+\eta_2^2)^2 + (\eta_3^2+\eta_4^2)^2] \\
& + g_{34}\,\eta_5(\eta_1^3 - 3\,\eta_1\,\eta_2^2 + \eta_3^3 - 3\,\eta_3\,\eta_4^2) \\
& + g_{44}\,\eta_5^2(\eta_1^2+\eta_2^2+\eta_3^2+\eta_4^2) + g_{54}\,\eta_5^4.
\end{aligned}
$$

Cubic term: 1st order transition

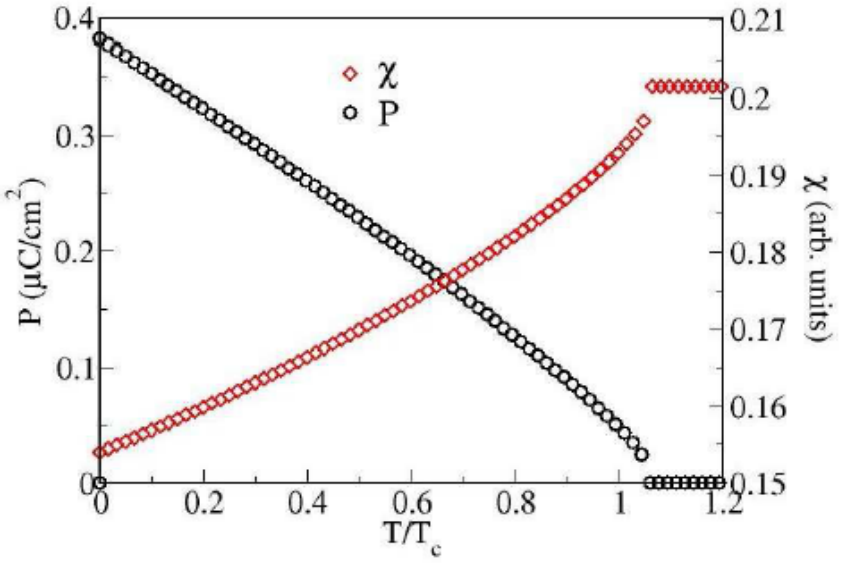
→ Nonlinear Coupling

Polarization induced as a *quadratic* function of Mo-trimerization:

P α $\eta_5 = -\frac{g_{23}}{2g_{22}}\eta_1^2$

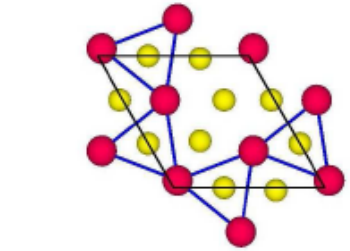
Ferroelectricity in MoS_2

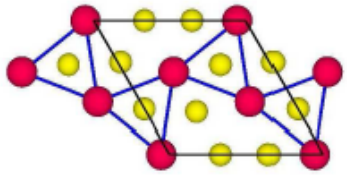
A

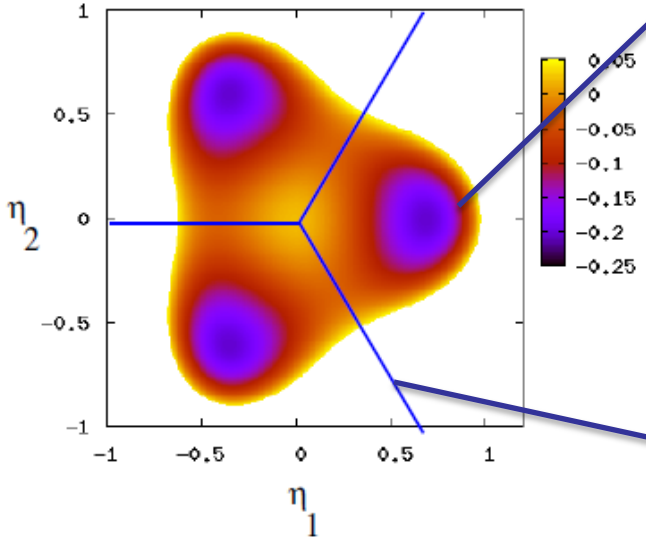


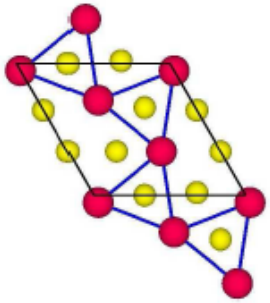
Dielectric anomaly:
IMPROPER FERROELECTRIC

B









Three Ferroelectric structures with the same P_z!

Lines of Metallic States

Our first-principles theoretical prediction:

1T-MoS_2 (with no electrodes):

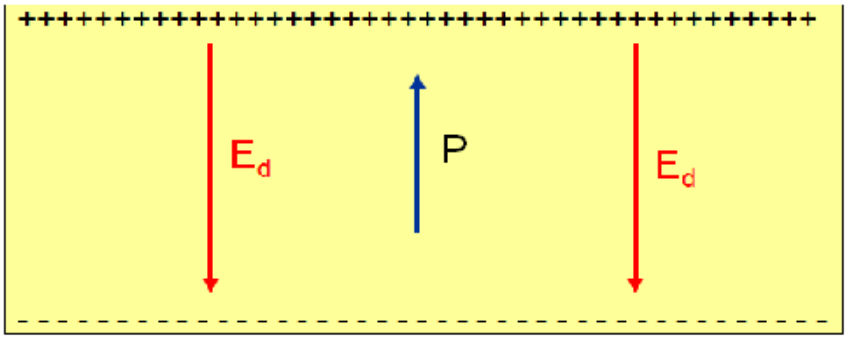
The world's thinnest known ferroelectric!

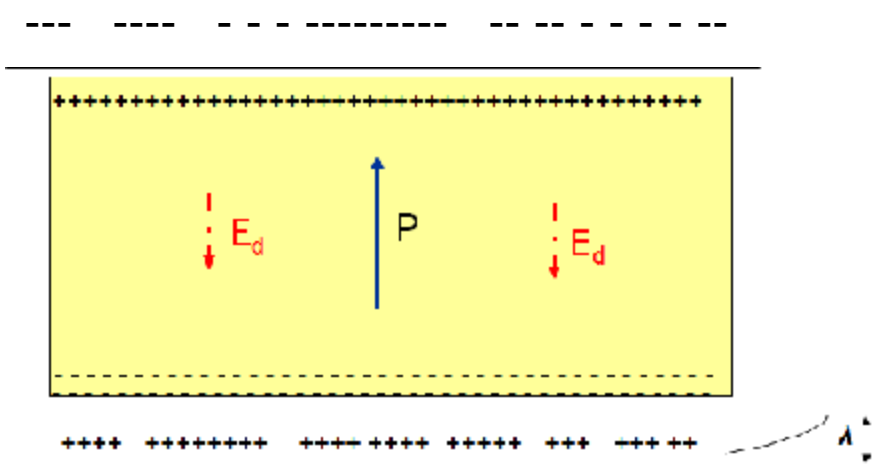
~ 0.6 nm

Other World Records (with electrodes):

1.0 nm: Polymer [PVDF] Bune et al, Nature 391, 874 (1998)

1.2 nm: $PbTiO_3$ Fong et al, Science 304, 1650 (2004).





1T MoS_2: 2D Ferroelectric Semiconductor

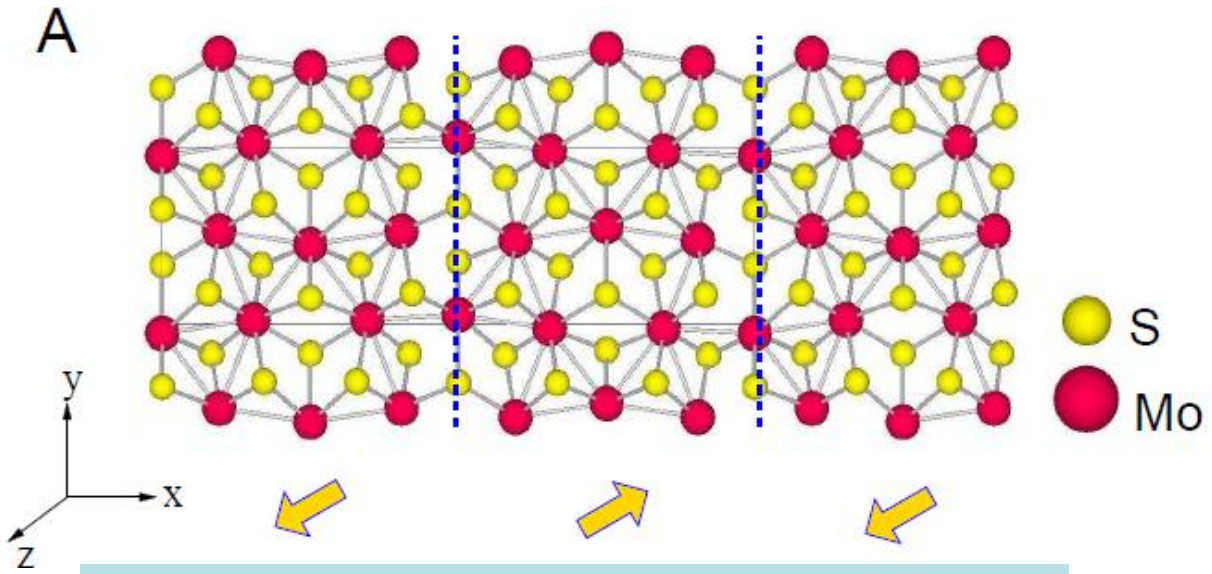
Electric dipole perpendicular to plane:
Bound charges, phonons

Electrical transport in-plane:
Free carriers

The two are strongly coupled!
Can we exploit this to make novel devices?

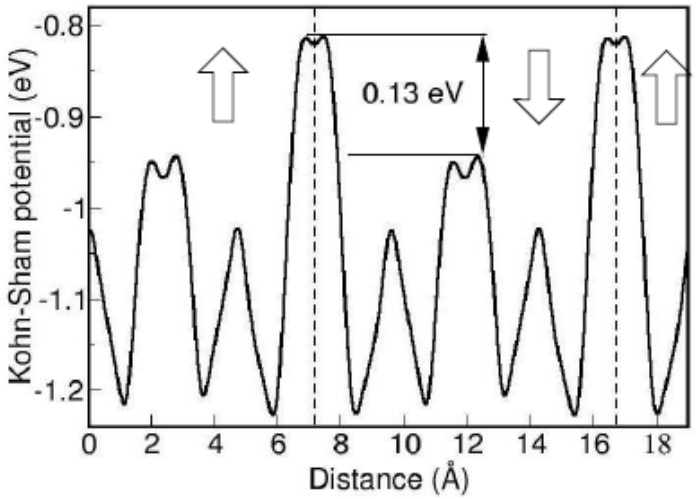
Ferroelectric Domains

Structure of Domain Walls



Domain Wall Energy of 7.7 mJ/m^2

Potential Energy Barrier at Domain Wall

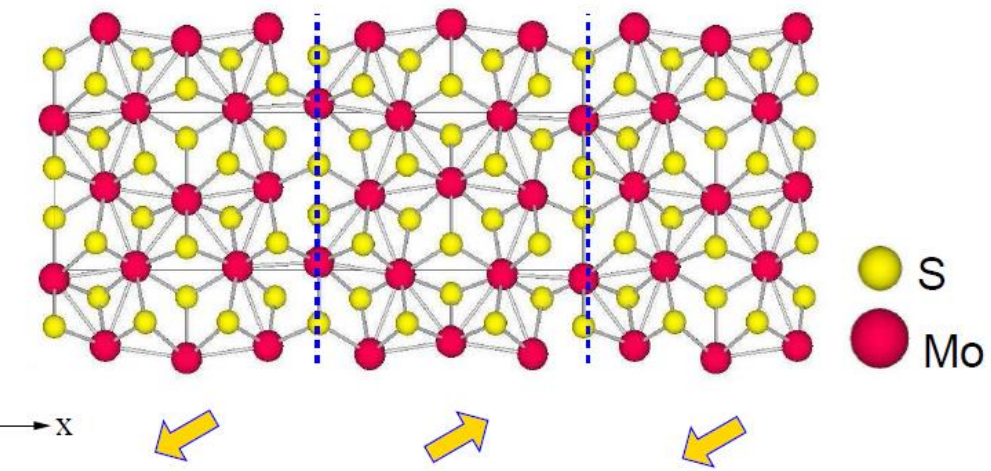


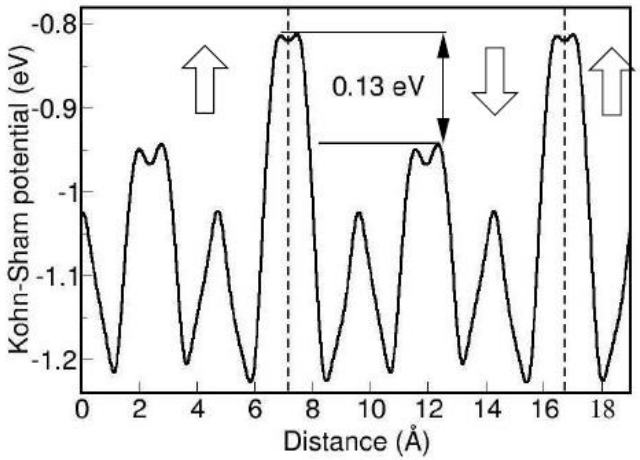
Domain Wall Energy Barrier of 0.13 eV:

Polarization switching:

Consequences to transport

Dipolectronic Devices based on MoS_2

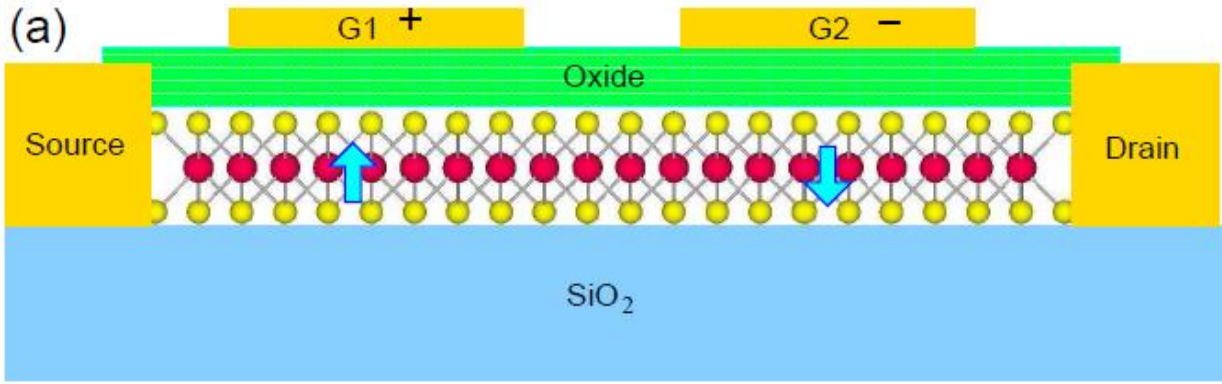




Coupled dipoles (bound) and Charge carriers (free)

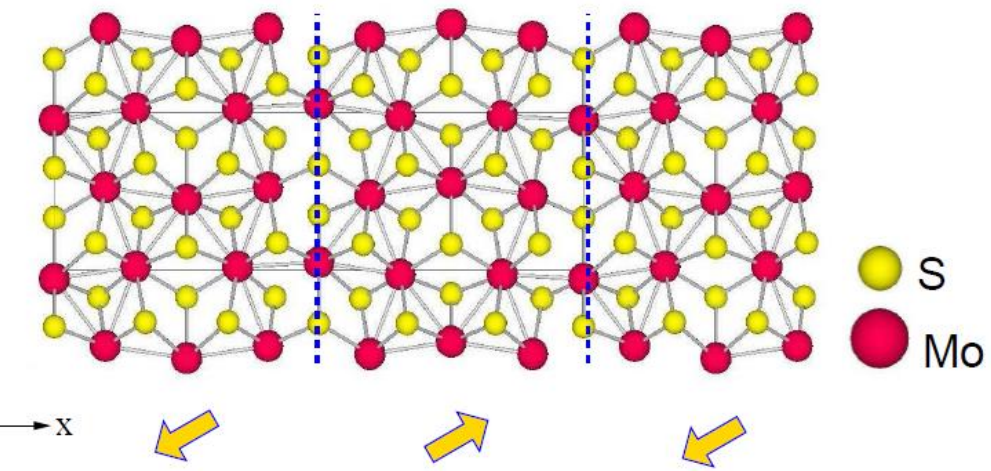
Control dipolar structure to control electric current

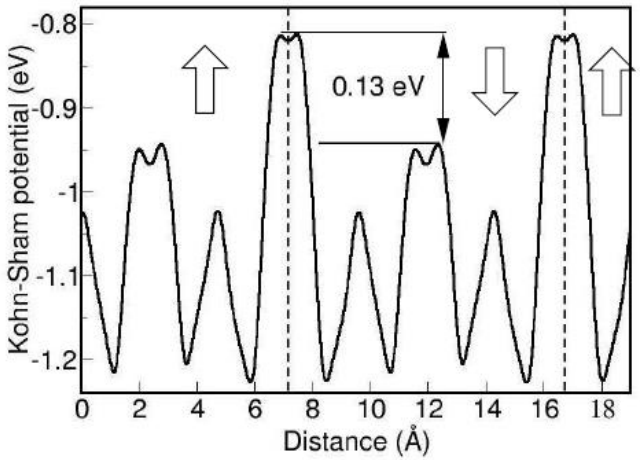
G1\G2	1	0
1	1	0
0	0	1



XNOR gate within a single device

Dipolectronic Devices based on MoS_2





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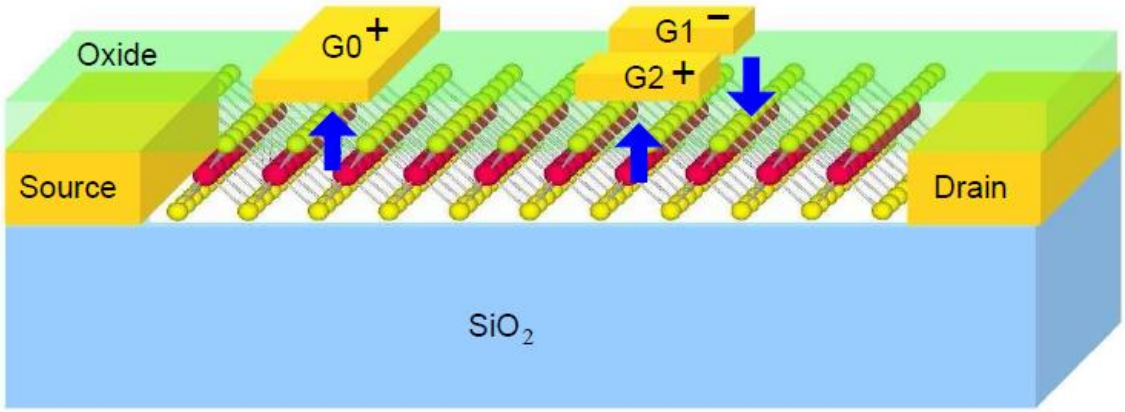
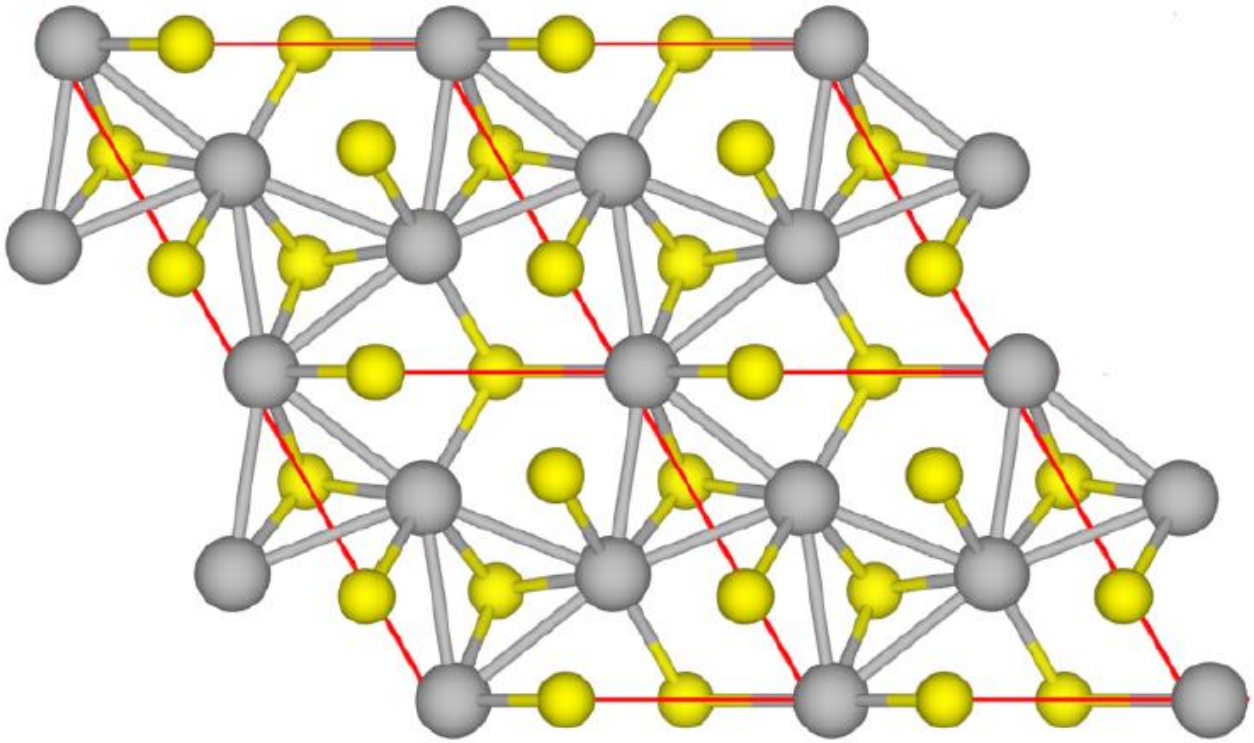


NAND gate within a single device

Symmetry Analysis, Ferroelectricity are generic to 1T polytype of $(Mo,W)(S,Se)_2$



Polarization ~ 0.25-0.28 μC/cm^2

But only MoS_2 has the stable domains and is usable!

Summary

Strong electron-phonon coupling and *its tunability with Electric Field:* generic to 2-D nanomaterials

Theoretical Demonstration of *Emergence of* **2-D** *ferroelectricity at an MIT* in *1T*-(Mo,W)(Se,S)$_2$

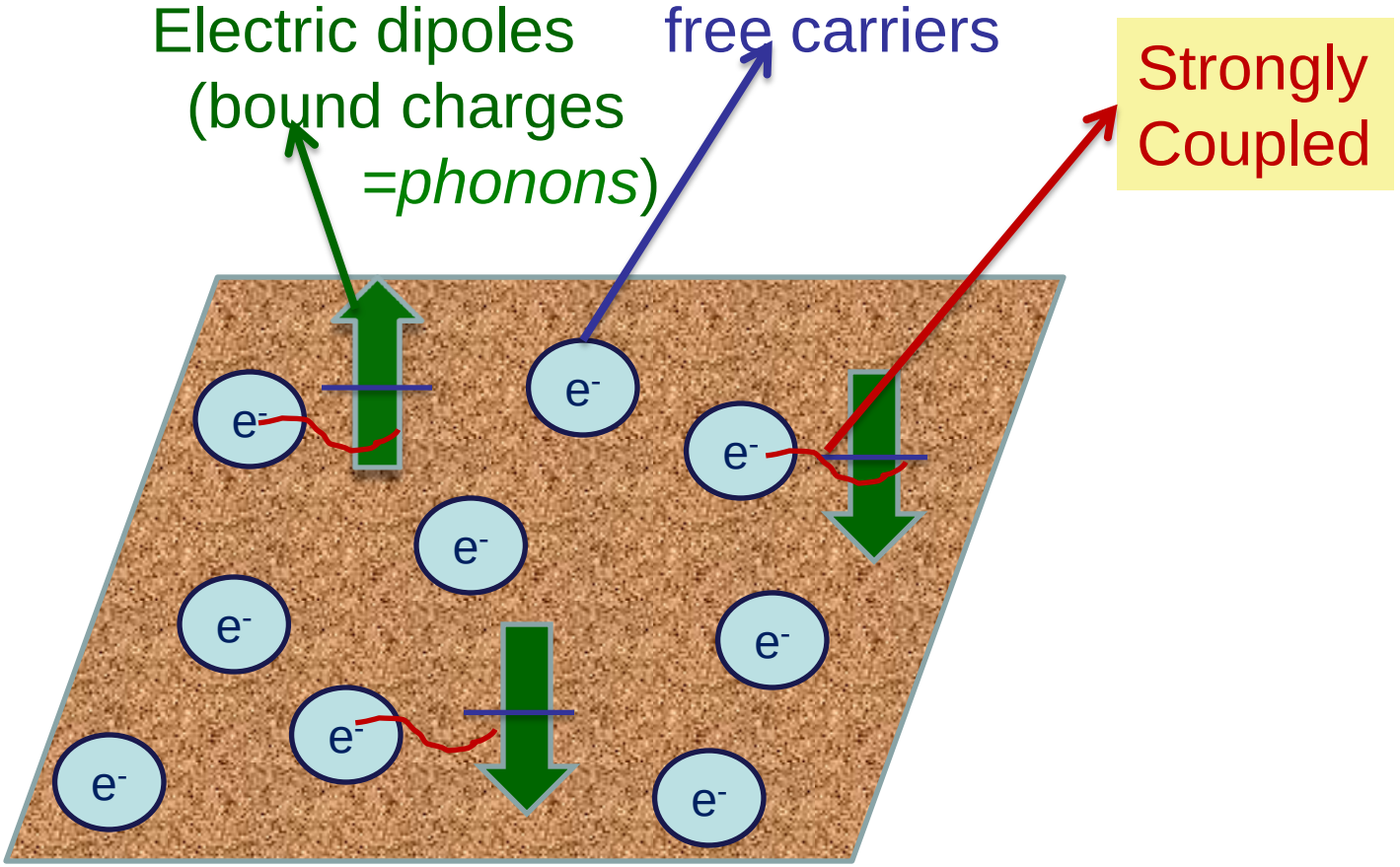
Origin: *electron-phonon coupling*

Dipolelectronic Devices

S N Shirodkar and U V Waghmare, Phys Rev Lett 112, 157601 (2014).

Take-Home Message: *1T MoS_2*

Ferroelectric Semiconductor



(nano)

Propose new class of devices: *Dipolectronics*

Why Phonons?

- Fingerprint of a material: Raman, IR spectra
- Thermodynamic stability: vibrational entropy T, soft modes
- Properties: elastic, dielectric, piezoelectric, etc (couple with fields)
- Structural Transitions: instabilities of a structure $w \rightarrow 0$
- Phonons coupled with electrons, spin, exciton, polarons; e.g. superconductivity

SiC

Ref. Thomas, Pandey and Waghmare, Phys Rev B (Rapid Comm), 77, 121203 (08)

SiC: a promising technological material both as a bulk and at nano-scale

(see a review by Melinon et al, Nature Materials 6, 479 (2007)).

Bulk SiC: mechanical hardness, optical properties (large band gap), bio-compatibility, high-temperature stability, chemical inertness, shock resistant, high refractive index

Stacking (eg. ABCAB...) of crystal planes **(polytypes)** tune properties

1950: Shockley predicted SiC would replace Si

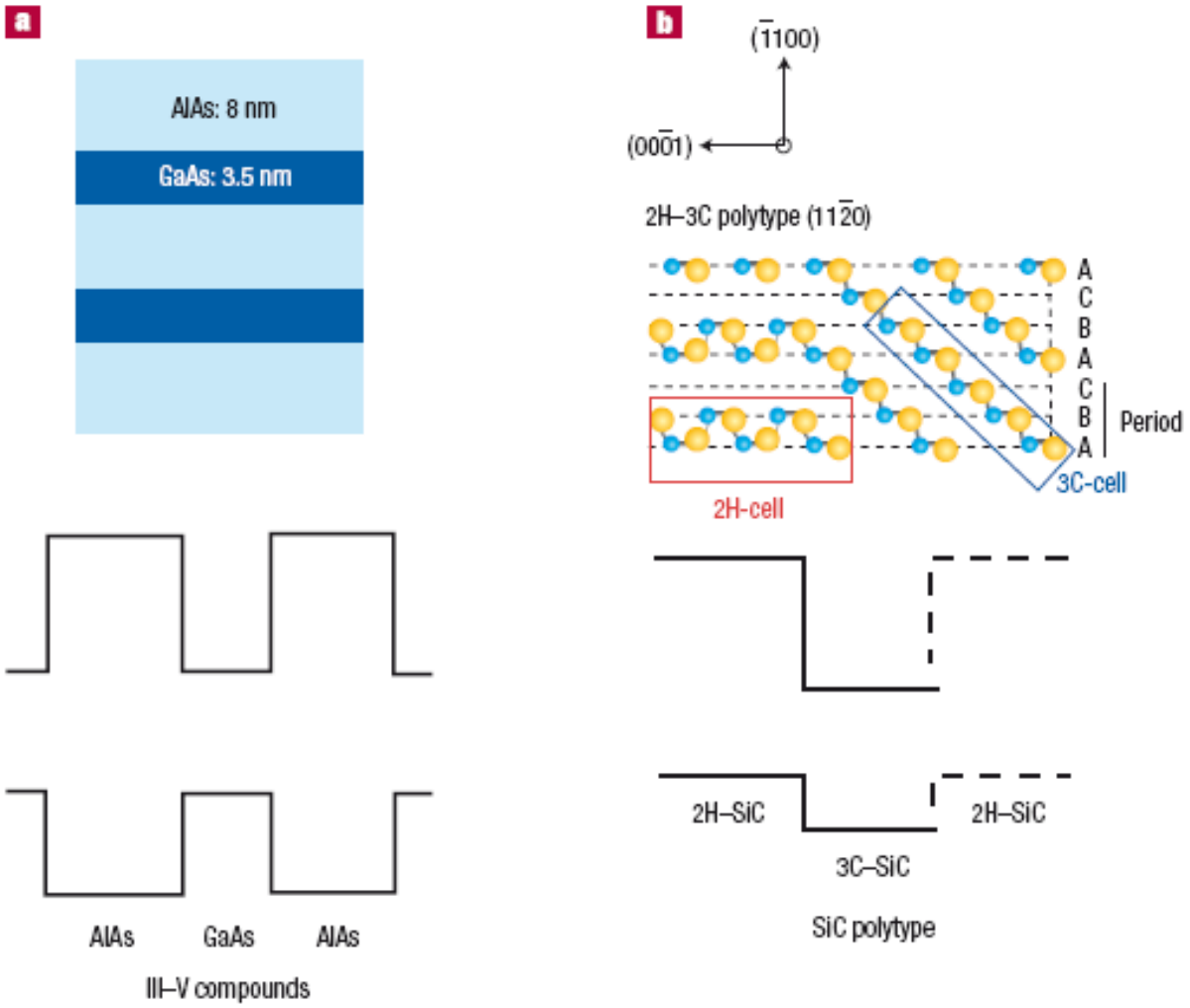
Many applications from power electronics to catalysis

Nano-form of SiC: Atomic engineering of nano-structures to tune properties

Clusters,

Nano-wires, nano-tubes,

Heterostructures



(From Nature Mat. 6, 479 (2007)).

Ultrahigh-quality silicon carbide single crystals

Daisuke Nakamura[1], Itaru Gunjishima[1], Satoshi Yamaguchi[1], Tadashi Ito[1], Atsuto Okamoto[1], Hiroyuki Kondo[2], Shoichi Onda[2] & Kazumasa Takatori[1]

[1]*Toyota Central R&D Laboratories, Inc., Nagakute, Aichi, 480-1192, Japan*
[2]*Research Laboratories, DENSO Corporation, 500-1, Nissin, Aichi, 470-0111, Japan*

Silicon carbide (SiC) has a range of useful physical, mechanical and electronic properties that make it a promising material for next-generation electronic devices[1,2]. Careful consideration of the thermal conditions[3–6] in which SiC {0001} is grown has resulted in improvements in crystal diameter and quality: the quantity of macroscopic defects such as hollow core dislocations (micropipes)[7–9], inclusions, small-angle boundaries and long-range lattice warp has been reduced[10,11]. But some macroscopic defects (about 1–10 cm^{-2}) and a large density of elementary dislocations (~10^4 cm^{-2}), such as edge, basal plane and screw dislocations, remain within the crystal, and have so far prevented the realization of high-efficiency, reliable electronic devices in SiC (refs 12–16). Here we report a method, inspired by the dislocation structure of SiC grown perpendicular to the *c*-axis (*a*-face growth)[17], to reduce the number of dislocations in SiC single crystals by two to three orders of magnitude, rendering them virtually dislocation-free. These substrates will promote the development of high-power SiC devices and reduce energy losses of the resulting electrical systems.

Nature 430, 1010 (2004)

Developed a method for making SiC crystals/wafers that have two to three orders of magnitude lower density of dislocations.

Repeated A-Face (RAF) growth:

At each stage, the crystal is carefully rotated so that the solidifying compound crystallises on the best, least-blemished face.

News Report on BBC

Last Updated: Wednesday, 25 August, 2004, 17:28 GMT 18:28 UK

Door open for silicon replacement

A replacement for the use of pure silicon in electronics has come a step closer, the journal Nature reports.
Silicon chips can malfunction at high temperatures, often from the heat generated in their own circuitry.

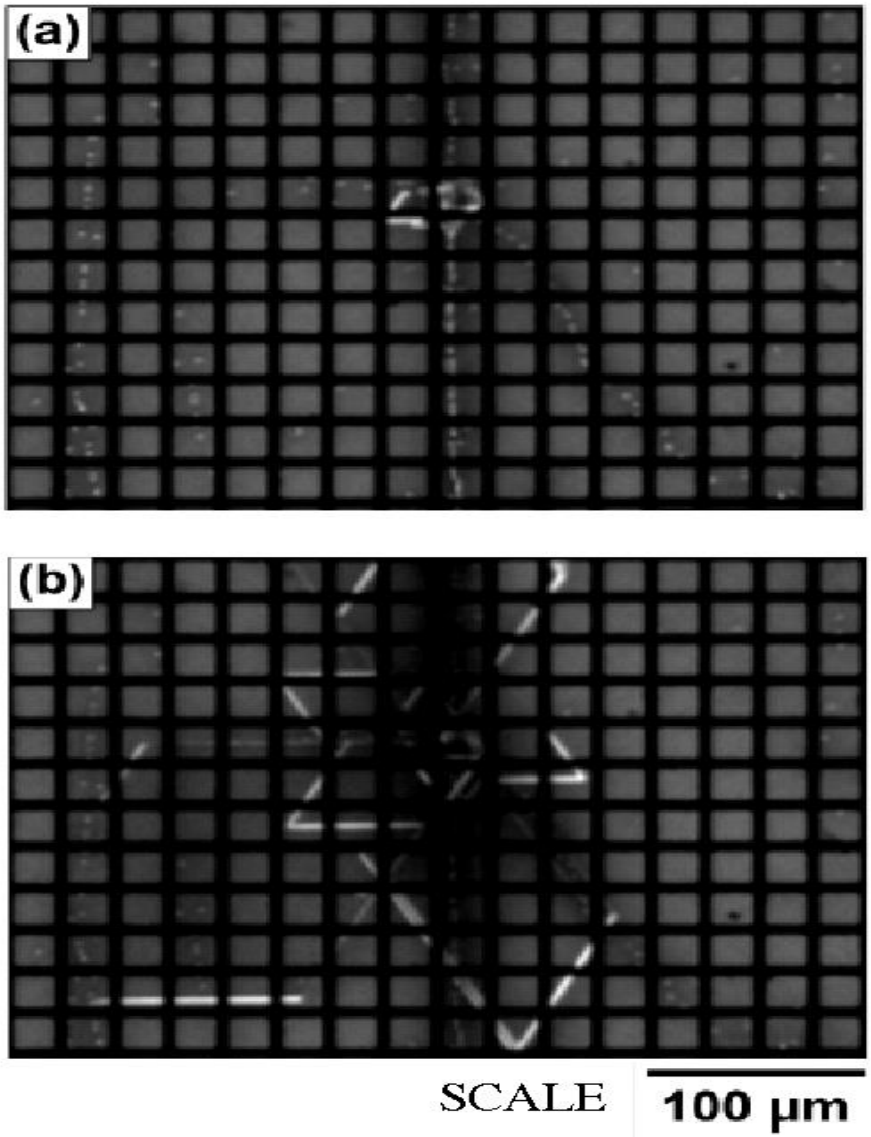
But Japanese experts have now overcome the flaws that plague crystals of silicon carbide, a hard compound that is more robust in hot conditions.

This material could now fulfil its potential as a replacement for pure silicon in manufacturing processes. Silicon carbide (SiC) could be used to make electronic devices that can operate at high power, in fierce heat or at lethal doses of radiation.

If the breakthrough can be carried forward commercially, it could spawn a wide range of improved devices, including electronics that work in red-hot jet engines, better wireless communications and radar, as well as improving smart devices that optimise performance in cars.

Problem: Stacking fault expansion in SiC

Ha, Skowronski, Sumakeris, Paisley and Das, Phy. Rev. Lett. 92, 175504 (2004)



OEM showing development of rhombic stacking faults in the basal plane of 4H-SiC when used in p-i-n diode

(a) Virgin diode

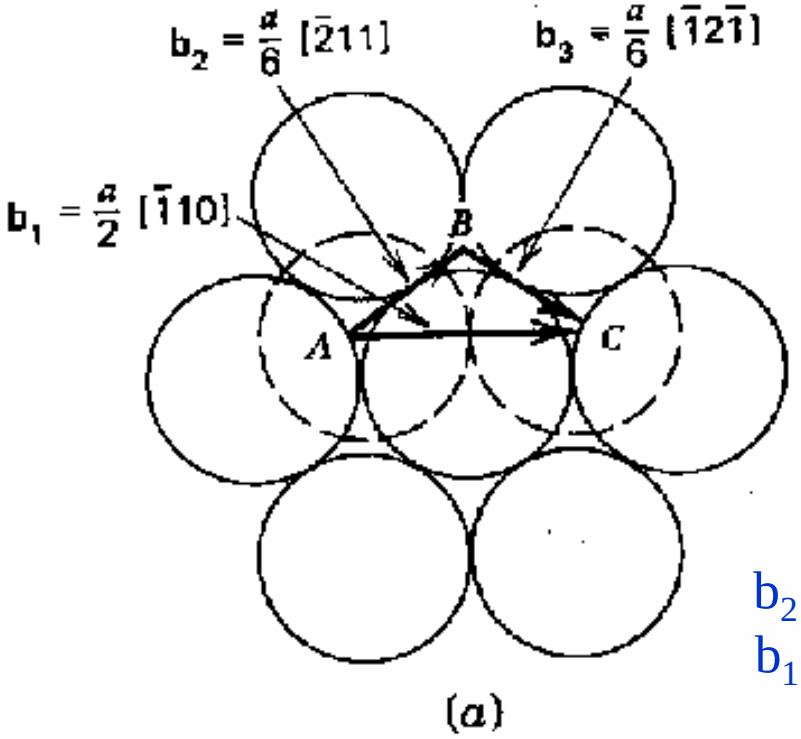
(b) Diode after 5 minutes of biasing at 50 A/cm^2

► Degraded performance: ΔV changes by up to 1 V!

Fundamental Problem

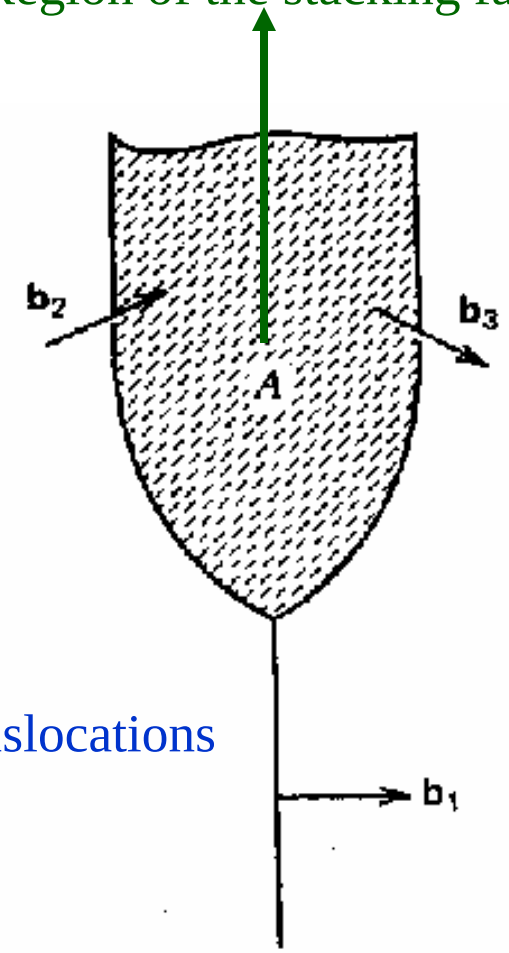
Origin of this phenomenon needs to be understood.

Stacking Faults



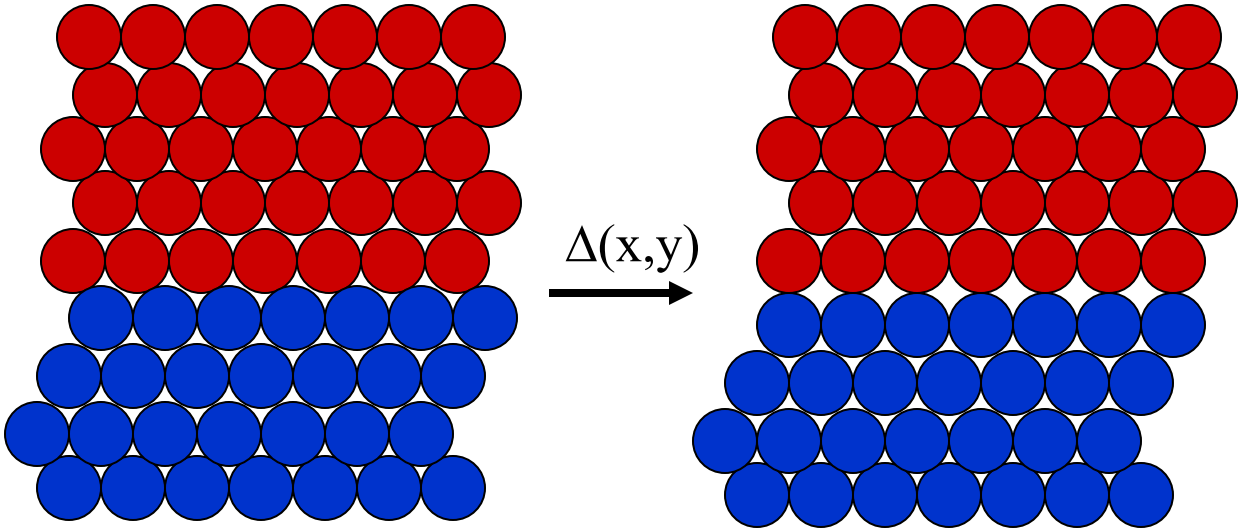
(a)

Region of the stacking fault



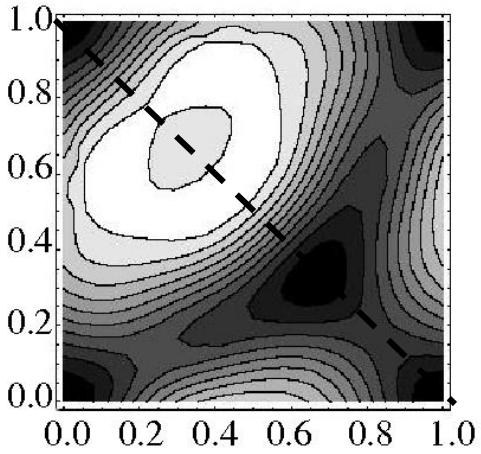
b_2 and b_3: partial dislocations
b_1: dislocation

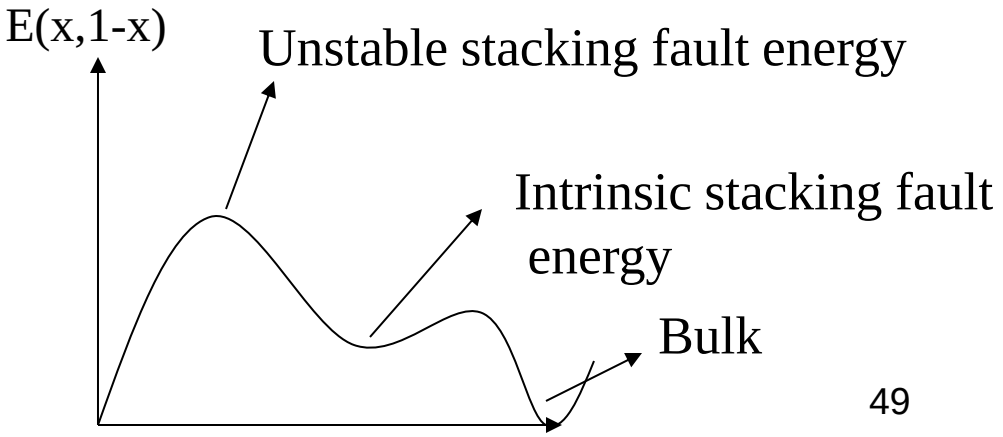
Generalized Stacking Fault Energy Surface
γ-surface: E(x,y)



1. Energy required to slip one half of a crystal with respect to the other by $x*a_1+y*a_2$
2. Exhibits periodicity of the unit cell (a_1,a_2) in the plane separating the two halves

Example:





Stacking fault expansion (T≠0): Statistical Thermodynamics

$$F = E + F_{config} + F_{vib}$$

Free energy of a crystal has 3 components:

(a) Internal energy: Total energy from DFT

(b) Configurational entropy: Obtain from the DFT γ-surface

Approximate energy basins in the γ-surface with

$$E(x,y) = E_o + K((x-x_o)^2 + (y-y_o)^2),$$

Free energy is then,

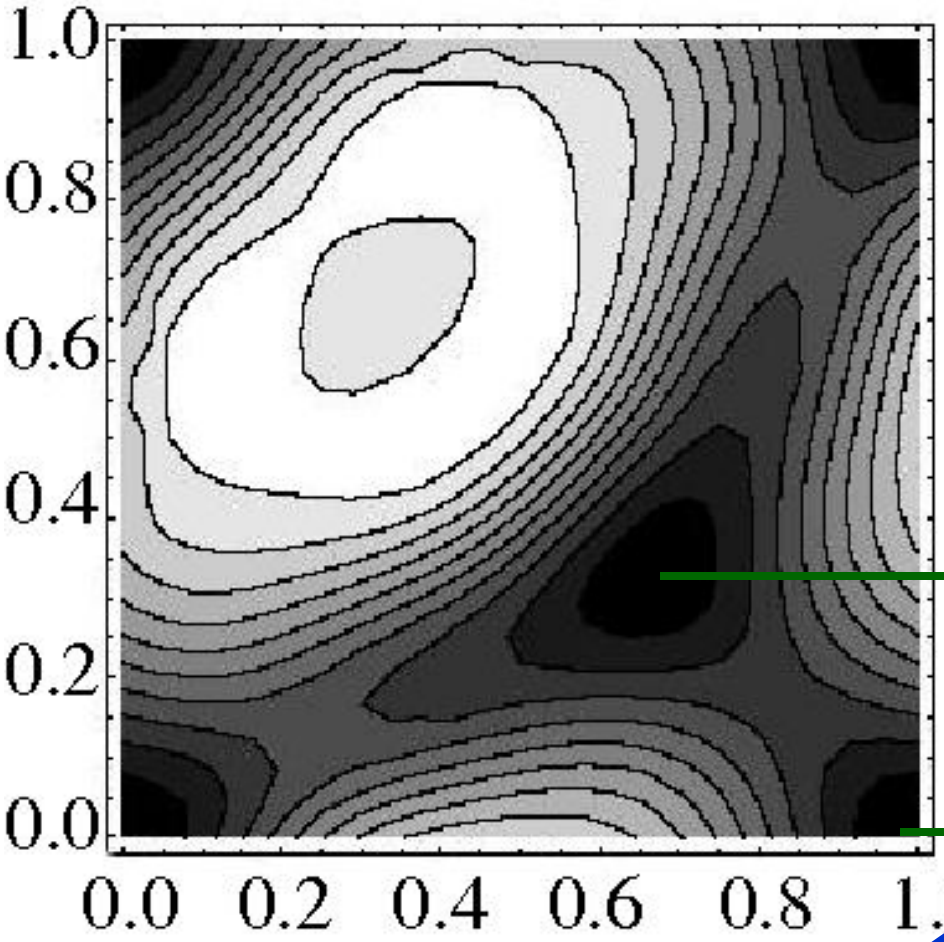
$$F_{conf} = -k_B T Log(\frac{K}{2\pi k_B T})$$

(c) Vibrational entropy: Obtain from phonons using DFT

$$F_{vib} = +k_B T \sum_{iq} Log(2sinh(\frac{\hbar\omega_{iq}}{2k_b T}))$$

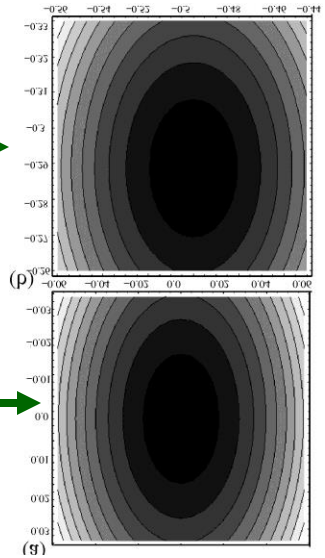
(a) Gives very low SFE (1 mJ/m^2) (earlier first-principles works).

The γ surface of 4H-SiC



Two energy basins :

(a) perfect (0,0) and
(b) faulted, (2/3,1/3)



(b)

(a)

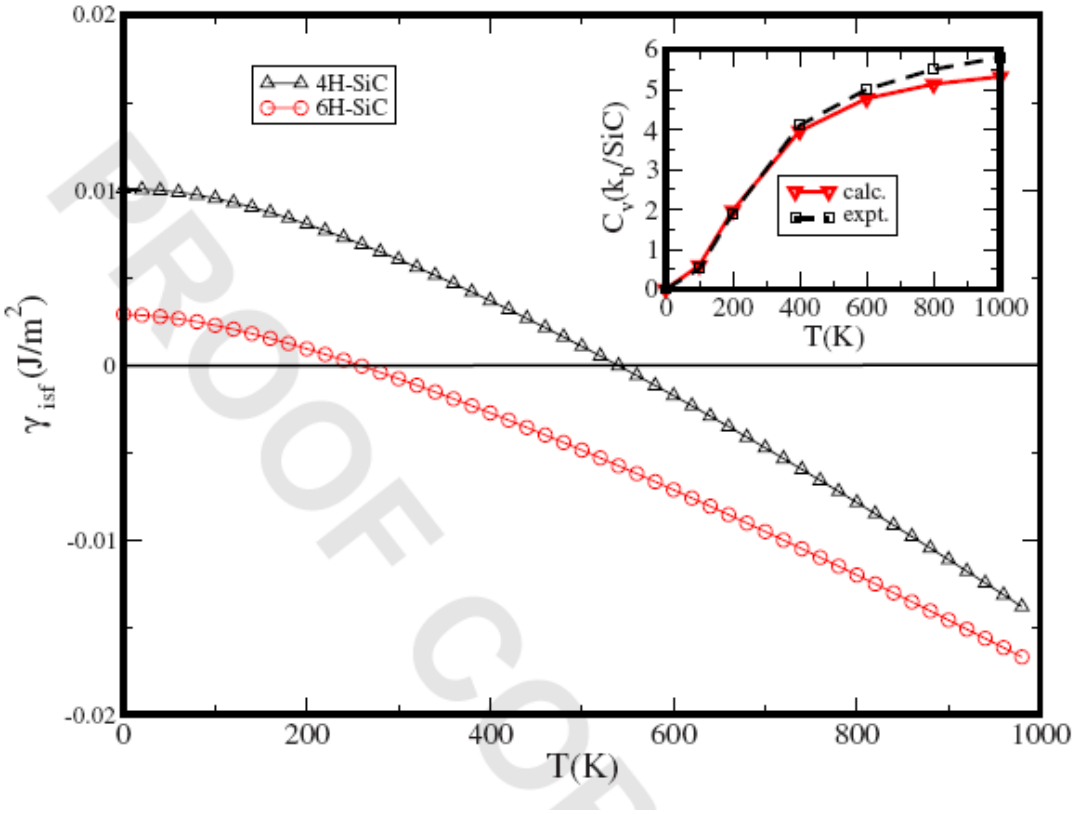
$$\gamma_s(T) = \gamma_s(0) + \Delta F_{conf}(T) + \Delta F_{vib}(T)$$

TABLE I. Calculated and experimental estimates of intrinsic (γ_{isf}) and unstable (γ_{us}) stacking fault energies for the slip in glide plane.

System	γ_{isf} (calculated) (mJ/m^2)	γ_{isf} (experimental) (mJ/m^2)	γ_{us} (J/m^2)
Si	46.9	69 (Refs. 26 and 27)	1.7
C	250	279 (Refs. 27 and 28)	5.5
Ge	48.5		1.6
3*C*-SiC	10.1		2.8
4*H*-SiC	9.1	14.7 ± 2.5 (Ref. 11)	2.9
6*H*-SiC	2.6	2.5 ± 0.9 (Ref. 12)	2.9

Ref. Thomas, Pandey and Waghmare, Phys Rev B (Rapid Comm), 77, 121203 (08)

Stacking fault energy of 4H-SiC



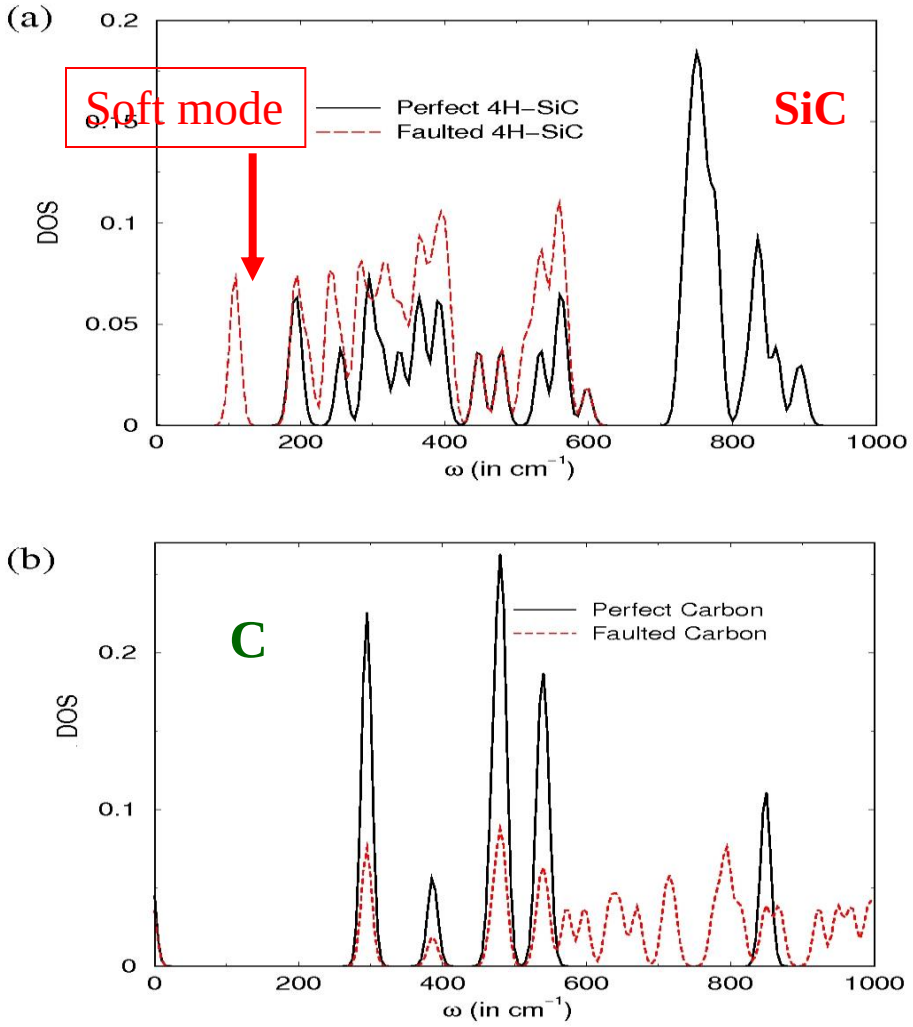
(1) Vibrational contribution to ΔF/T of (0.2×10-3 J/m^{2}K) dominates over the configurational contribution of (0.27×10-5 J/m^{2}K).

(2) γs(T) <0 for T > 60 K

► the faulted structure stabilized,
yielding the observed stacking fault expansion.

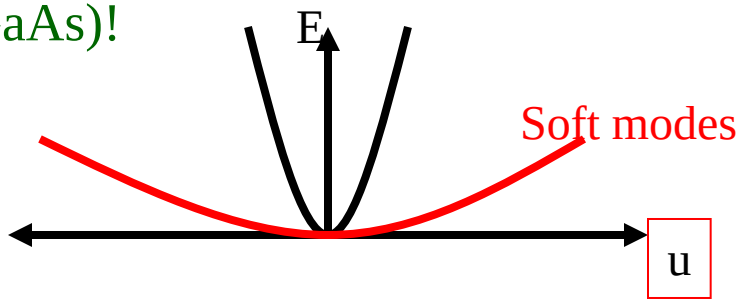
Origin of Observed Stacking Fault Expansion in 4H-SiC

Phonon DoS



Soft modes at 107.3, 107.4, 109.9 and 110.0 cm^{-1} in faulted 4H-structure of SiC

No such modes in Carbon (or Si, Ge, GaAs)!

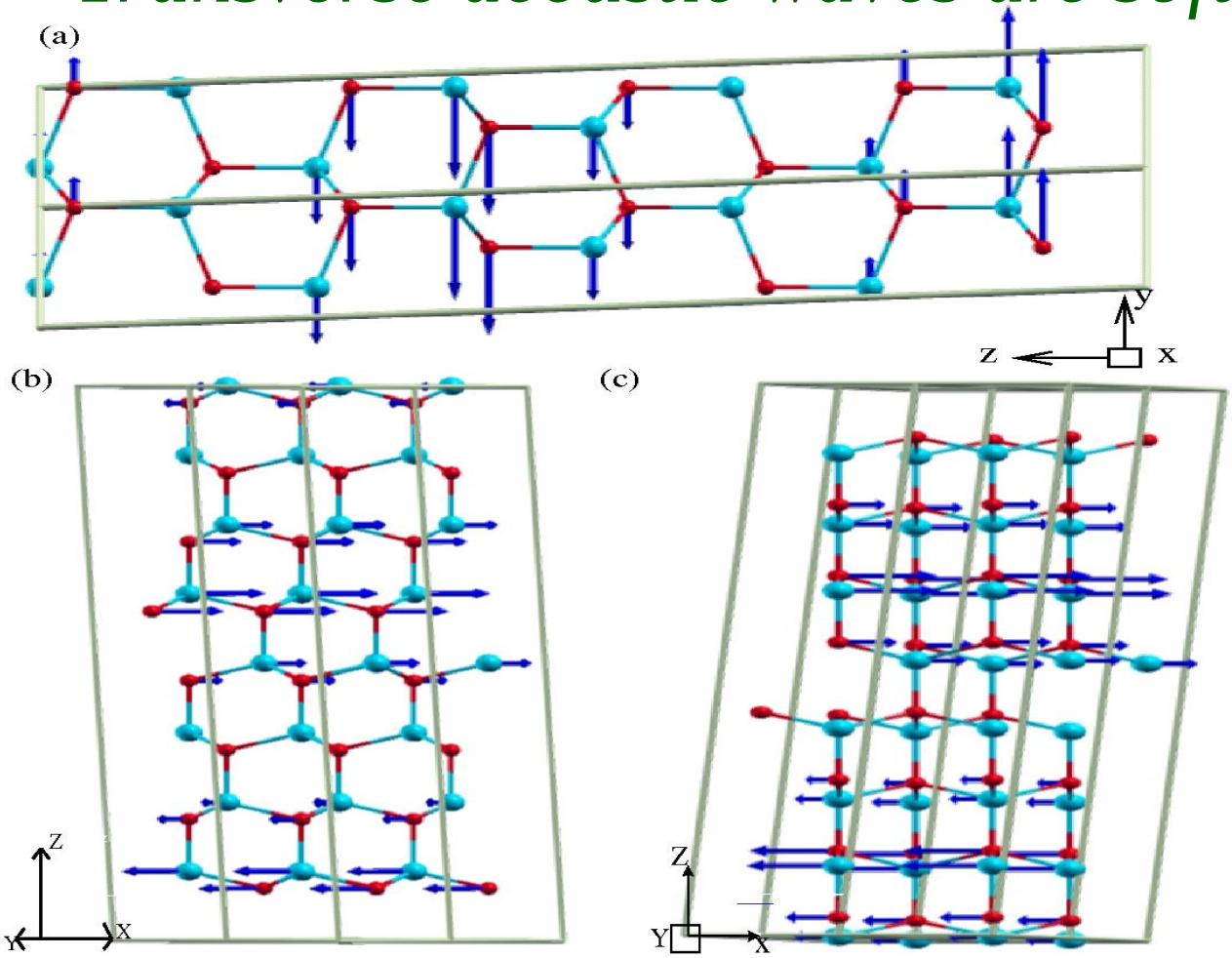


Soft modes: greater entropy

Soft phonon modes commonly responsible for structural phase transitions in solids. Here, we discover them in the context of stacking fault expansion.

Soft modes: Shear straining

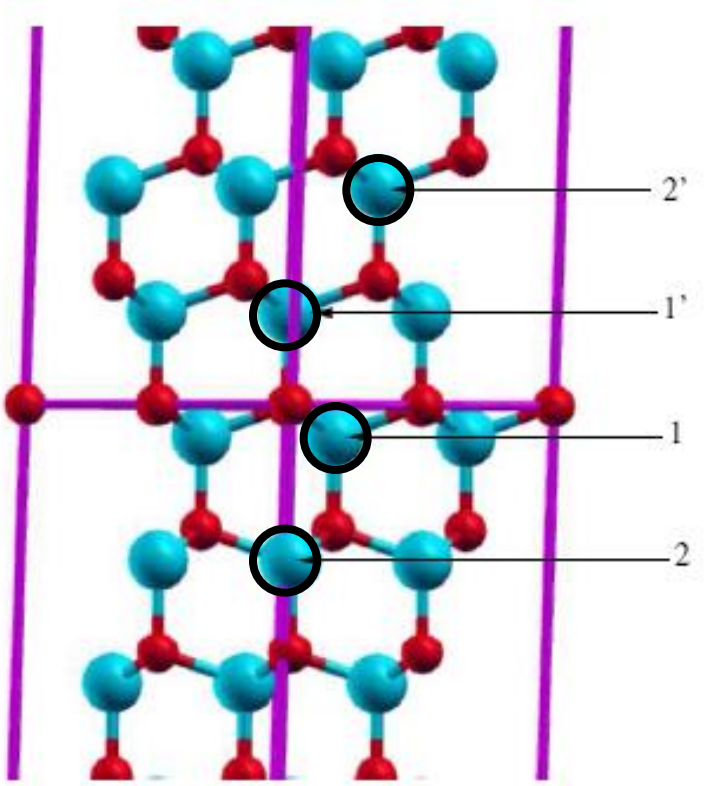
Transverse acoustic waves are softened



Prediction to be verified experimentally: *Shear waves will be slown down.*

Can we stop the stacking fault expansion in SiC?

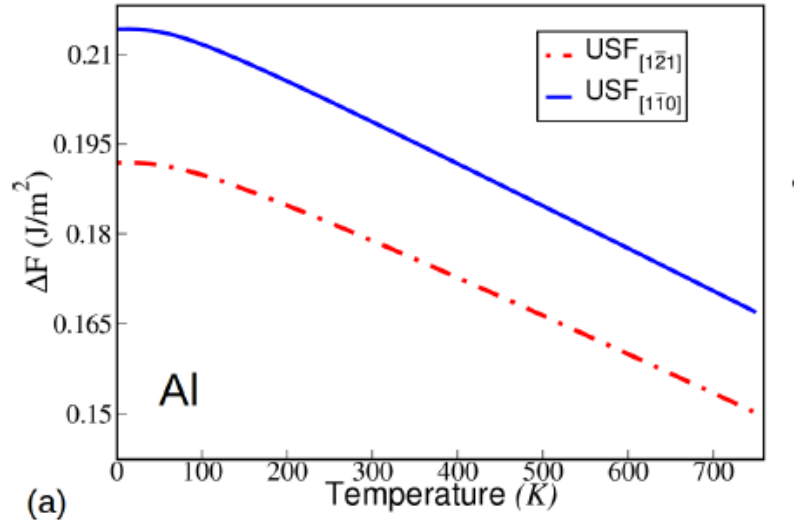
► *Through suitable substitutional doping to arrest it!*

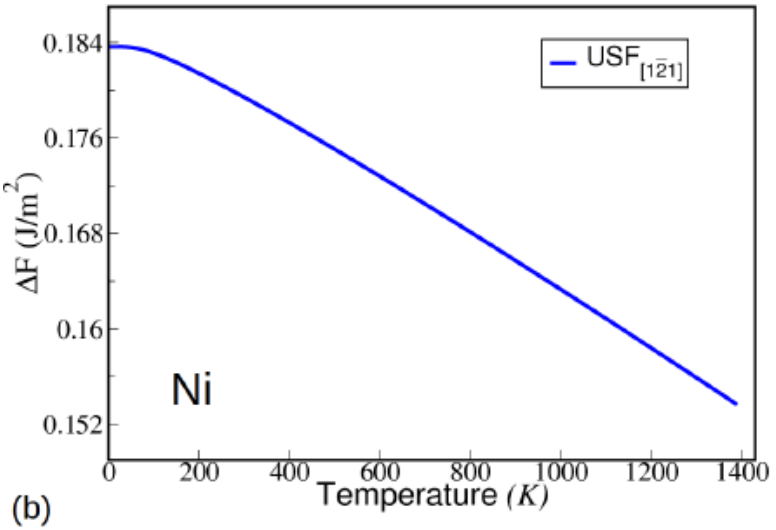


V and Cr doping in SiC results in higher SF energies, while also giving a DMS!

	TM	N	Fault (y/n)	Energy (meV) FM	Energy (meV) AFM	J (meV)	γ_{sf} (mJ/m^2) FM	γ_{sf} (mJ/m^2) AFM
6H	Cr	1	y	34.0	194.7	-160.7	16.6	35.5
			n	0.0	121.8	-121.8		
	Cr	2	y	253.2	261.1	-7.9	2.3	6.2
			n	245.2	248.3	-3.1		
	Cr	3	y	279.2	279.3	-0.1	24.9	24.6
			n	228.0	228.7	-0.7		
	Mn	1	y	0.0	57.1	-57.1	-62.1	-8.4
			n	127.4	74.3	53.1		
	Mn	2	y	335.0	335.0	0.0	18.8	17.2
			n	296.5	299.6	-3.1		
	Mn	3	y	358.1	357.6	0.5	29.2	28.0
			n	298.1	300.1	-2.0		
	V	1	y	38.0	—	—	18.5	—
			n	0.0	—	—		
	V	2	y	372.5	377.7	-5.2	15.8	12.3
			n	340.0	352.5	-12.5		
	V	3	y	387.5	399.7	-12.2	20.2	22.2
			n	346.1	354.0	-7.9		

Unstable Stacking Fault Energies in Metals





Energy release rate
for nucleation of dislocations

20-25 % reduction as
T increases to 0.8 T_m

In Cu, the configuration is
unstable!

Enhanced ductility

Bhogra, Ramamurty and Waghmare, JPCM (2014)

Why Phonons?

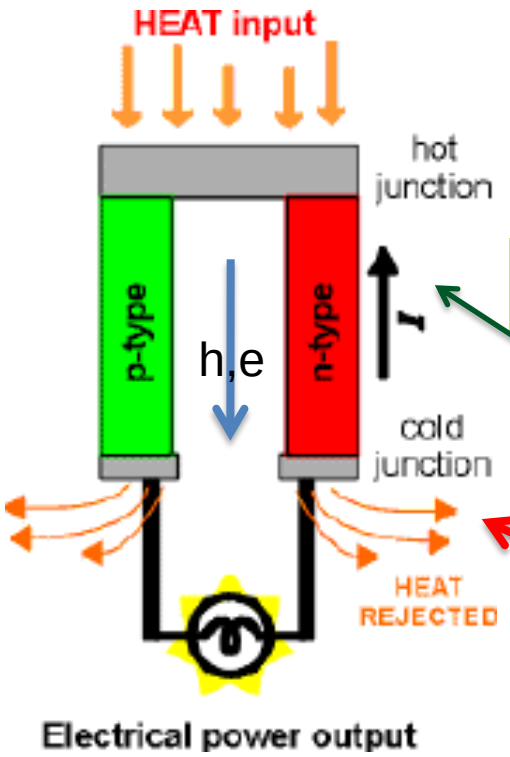
- Fingerprint of a material: Raman, IR spectra
- Thermodynamic stability: vibrational entropy T, soft modes
- *Properties: elastic, dielectric, piezoelectric, etc (couple with fields)*
- Structural Transitions: instabilities of a structure $w \rightarrow 0$
- Phonons coupled with electrons, spin, exciton, polarons; e.g. superconductivity

Thermoelectrics and energy conversion

Directly convert thermal energy to electrical energy

Environmentally friendly, No moving parts (except for a fan)

Seebeck Effect:



$\Delta V = S\,\Delta T$

Figure of Merit:

$$ZT = \frac{S^2 \sigma}{k_e + k_p} T$$

It should carry electric current, but NOT heat (dominated by phonons)

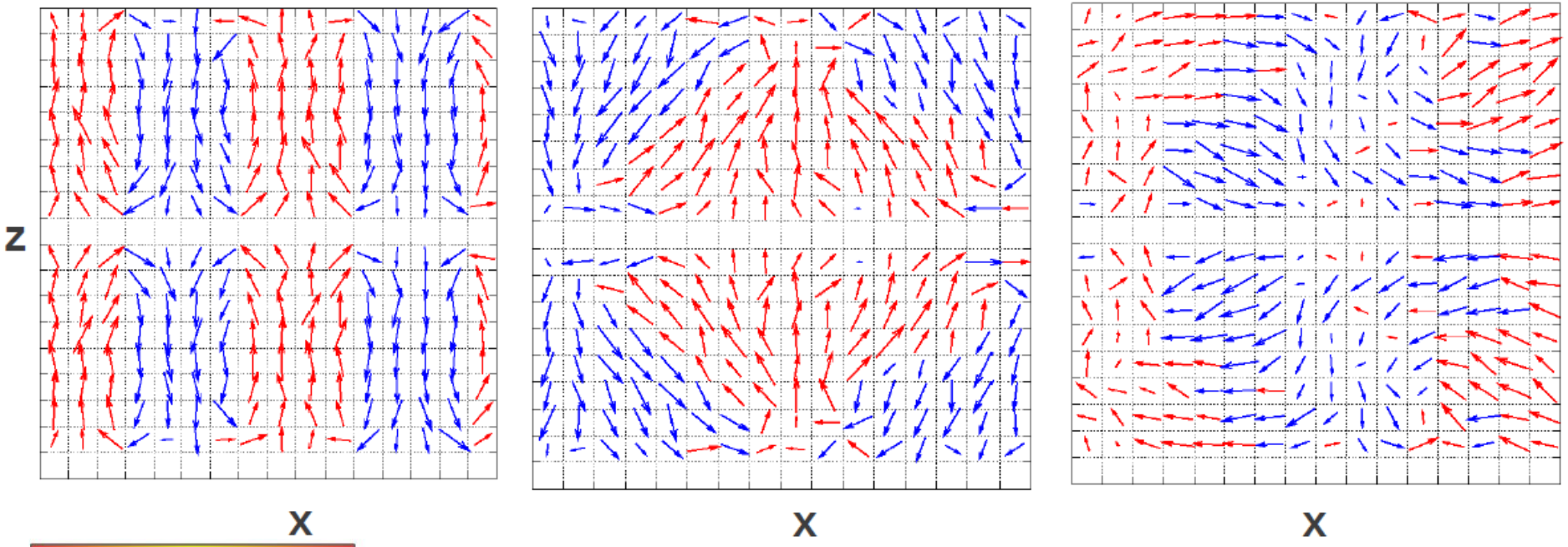
A key to designing high ZT materials is to *manipulate* transport of phonons and electrons*: low k*

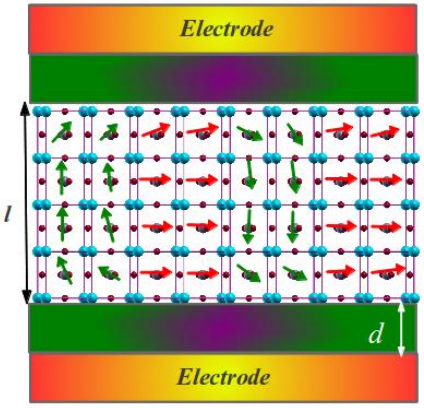
Properties of Ferroelectric Domains

Strain Engineering of Domain Structure in epitaxial $PbTiO_3$

Compressive → Tensile

η = -0.02 | η = -0.005 | η = 0.01

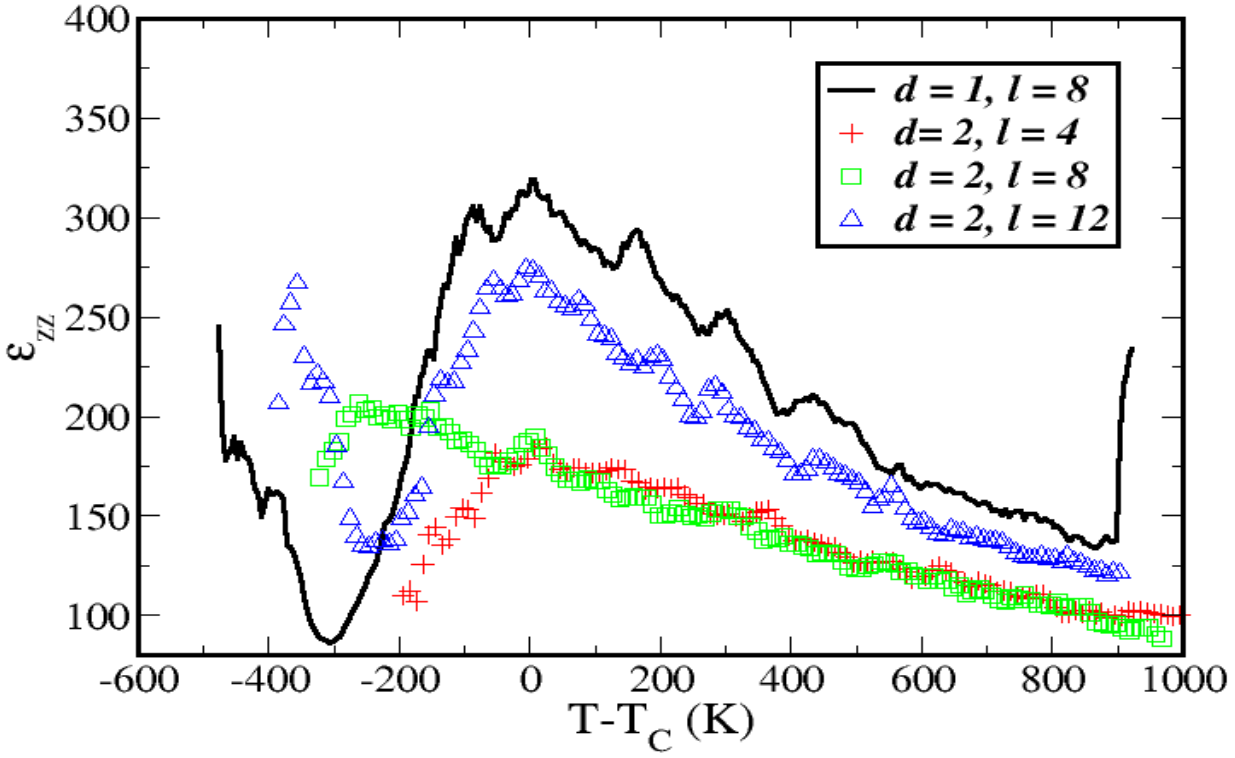




Imperfect electrodes influence ordering of polar phonons

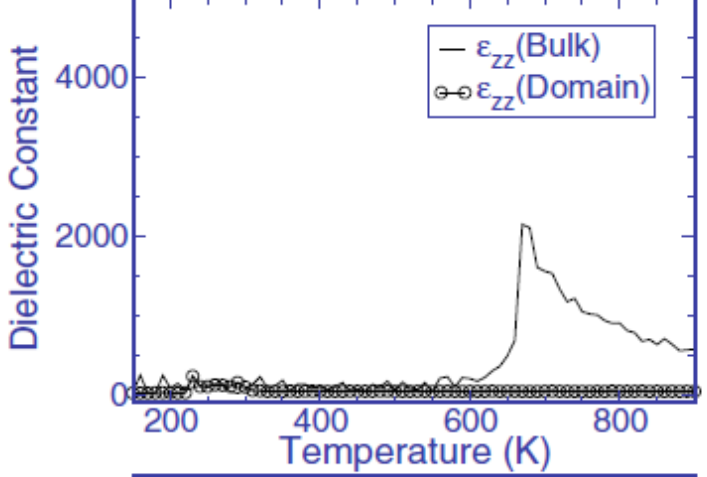
Kouser, Nishimatsu, Waghmare,
Phys. Rev. B **88**, 064102 (2013); PRB Kaleidoscope, Aug (2013)

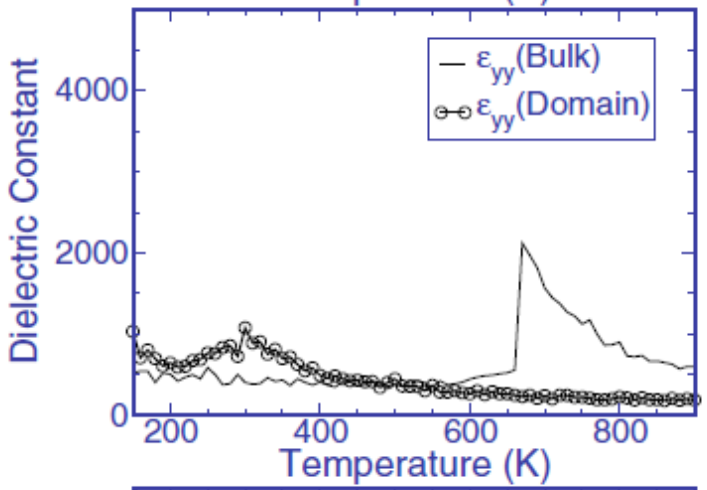
Diffuse Dielectric Response of Domain Structure ($PbTiO_3$)

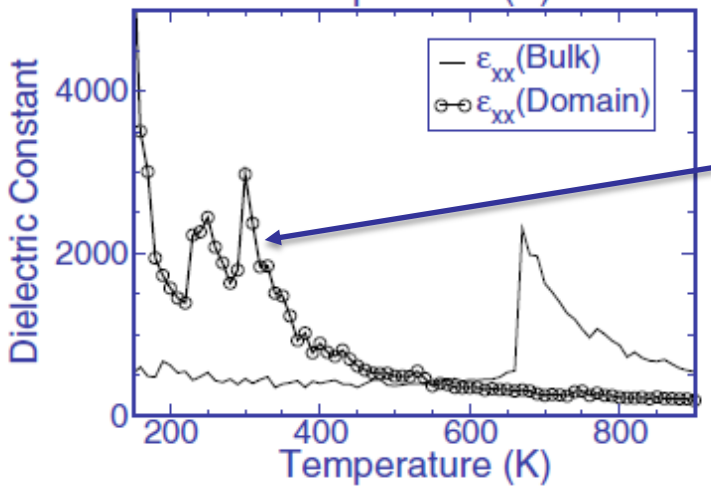


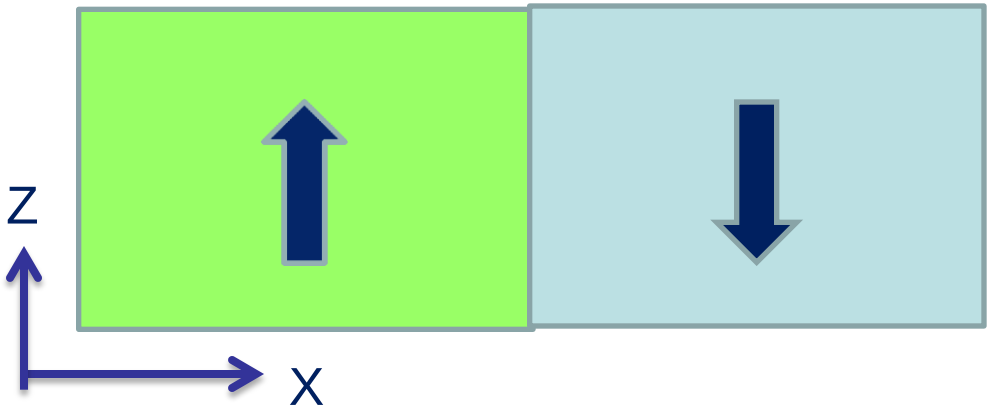
Ordering to inhomogeneous phase leads to a diffuse dielectric response across the transition

Dielectric Response of a 180° Ferroelectric Domain in $PbTiO_3$





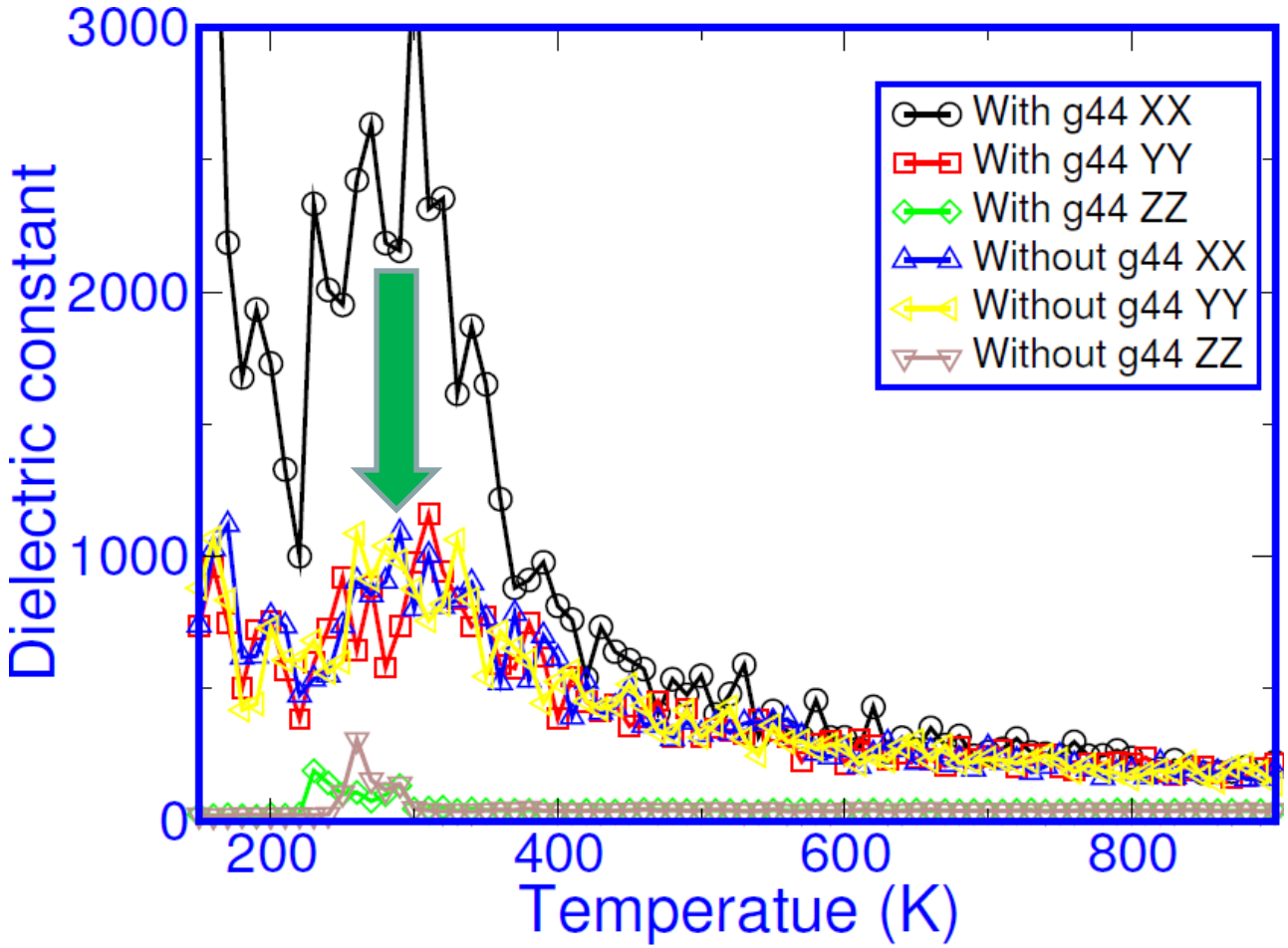




Enhanced Dielectric Response
In the direction perpendicular to the domain wall!

Why xx component?

Corroboration of the phen. Theory from MD



Strain-phonon coupling: dielectric response of a domain wall

Collaborators

Sharmila N Shirodkar
Anjali Singh
Tiju Thomas
Summayya Kouser
T Nishimatsu

D Pandey (BHU)

Thank you!