$LaMnO_3$ Revisited

A Comprehensive First-Principles Study of the Interplay Between Strain, Lattice mode, and Electronic Degrees of Freedom

Michael-Marcus Schmitt,Yajun Zhang, Alain Mercy, Eric Bousquet, & Philippe Ghosez

XXIVth International Symposium on the Jahn-Teller Effect
24th-29th June 2018 - Santander

Physique Théorique des Matériaux, Q-MAT, CESAM, Université de Liège

Outline

- (Re)classifying Cooperative Jahn-Teller Distortions in Perovskites

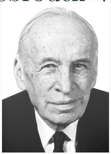
- $LaMnO_3$
  - Bulk
  - Epitaxial Thin Films

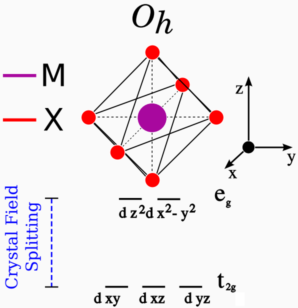
- An Approach to a Ferromagnetic/Ferroelectric Multiferroic $RMnO_3$ Compound

(Re)classifying Cooperative Jahn-Teller Distortions in Perovskites

Van Vleck: The octahedral Complex MX_6

John Hasbrouck Van Vleck





Van Vleck, J. H. The Journal of Chemical Physics 7.1 (1939): 72-84.

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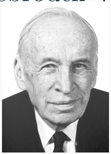
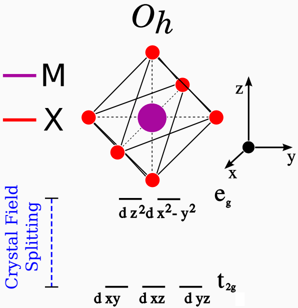


$$\mathbf{e_g} \otimes \mathbf{e_g} = \mathbf{a_{1g}} + \mathbf{e_g}$$



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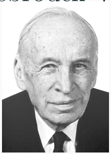
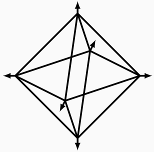


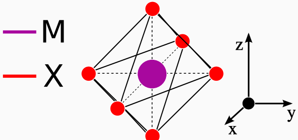
$$\mathbf{e_g} \otimes \mathbf{e_g} = \mathbf{a_{1g}} + \mathbf{e_g}$$

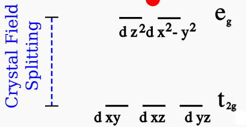
$\mathbf{a_{1g}}$

Q_1



O_h





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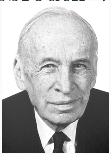

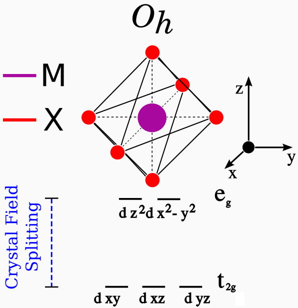

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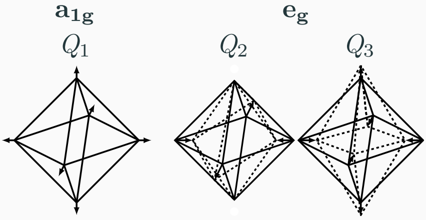

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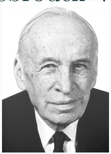
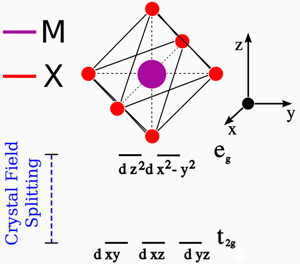


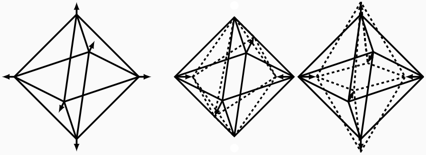
O_h



$$\mathbf{e_g} \otimes \mathbf{e_g} = \mathbf{a_{1g}} + \mathbf{e_g}$$

$\mathbf{a_{1g}}$ $\mathbf{e_g}$

Q_1 Q_2 Q_3



$$\mathbf{t_{2g}} \otimes \mathbf{t_{2g}} = \mathbf{a_{1g}} + \mathbf{e_g} + \mathbf{t_{2g}}$$

Van Vleck, J. H. The Journal of Chemical Physics 7.1 (1939): 72-84.

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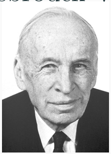
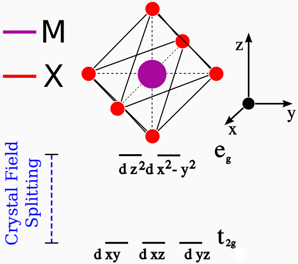


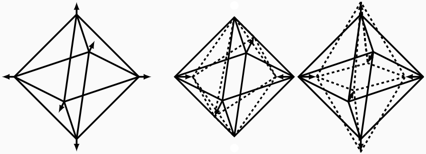
O_h



$$\mathbf{e_g \otimes e_g = a_{1g} + e_g}$$

$\mathbf{a_{1g}}$ $\mathbf{e_g}$

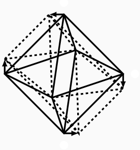
Q_1 Q_2 Q_3



$$\mathbf{t_{2g} \otimes t_{2g} = a_{1g} + e_g + t_{2g}}$$

$\mathbf{t_{2g}}$

Q_4, Q_5, Q_6



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$$\mathbf{e_g} \otimes \mathbf{e_g} = \mathbf{a_{1g}} + \mathbf{e_g}$$

Many different Notations for this in the literature!

Chemists

$$Q_\theta, Q_\epsilon$$

O'Brien, M. C. & Chancey, C. Am. J. Phys., 1993, **61**, 688-697

Labels of Irreducible Representation

M2+, M3+, R3-, R3+, R4-...

Carpenter, M. A. & Howard, C. J. Acta Crystallogr. B., 2009, **65**, 134-146

Solid State Physicists

$$Q_1^M, Q_1^R, Q_2^+, Q_2^-, M_{JT}, R_{JT}, Q^x, Q^z, Q_R^x, Q_R^z ...$$

He, Z. & Millis, A. J. Phys. Rev. B, 2015, **91**, 195138

Varignon, J.; Bristowe, N. C. *et al.*; Sci. Rep., 2015, **5**, 15364

Varignon, J.; Bristowe, N. C. & Ghosez, P. E Phys. Rev. Lett., 2016, **116**, 057602

Ederer, C.; Lin, C. & Millis, A. J. Phys. Rev. B, 2007, **76**, 155105

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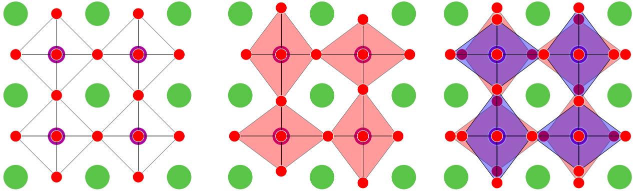
Chemists

Perovskite Structure



Same Individual Distortion

Through Different Cooperative Arrangements

Varignon, J.; Bristowe, N. C. & Ghosez, P. E Phys. Rev. Lett., 2016, **116**, 057602

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$$\mathbf{e_g} \otimes \mathbf{e_g} = \mathbf{a_{1g}} + \mathbf{e_g}$$

Many different Notations for this in the literature!

A Revised Notation!

i = Vlecks Numbering   q = q-vector in Cubic BZ

$$Q_i^q$$

i	$Q_i \cdot e^{i\vec{q}\vec{x}}$
1	$\Gamma = (0,0,0) = Strain$
2	$X = (\pi, 0, 0)$
3	$M = (\pi, \pi, 0)$
4	$R = (\pi, \pi, \pi)$

He, Z. & Millis, A. J. Phys. Rev. B, 2015, **91**, 195138

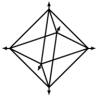
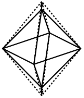
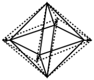
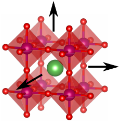
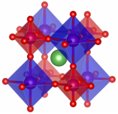
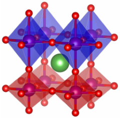
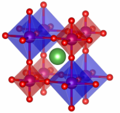
Kanamori, J. J. Appl. Phys., 1960, **31**, 14-23

Varignon, J.; Bristowe, N. C. & Ghosez, P. E Phys. Rev. Lett., 2016, **116**, 057602

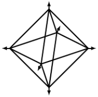
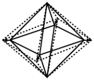
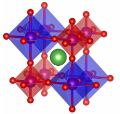
Ederer, C.; Lin, C. & Millis, A. J. Phys. Rev. B, 2007, **76**, 155105

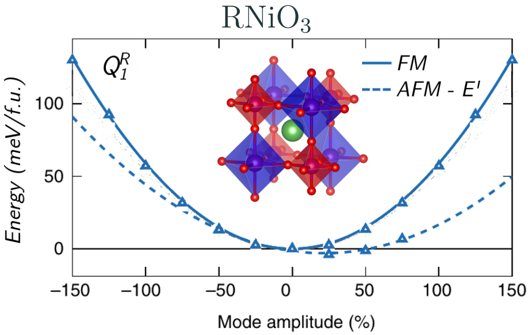
Van Vleck, J. H. The Journal of Chemical Physics 7.1 (1939): 72-84.

Q_1-Modes and Strains

Q_1 	Q_1^{Γ}	$Q_1^{\mathbf{R}}$	$Q_1^{\mathbf{X}}$ 	$Q_1^{\mathbf{M}}$ 
Origin in A	$\Gamma 1+$ (a)	$R2-$ (a)	$X3-$ $(a,0,0)$	$M4+$ $(a,0,0)$
Ref. $Pm\overline{3}m$ B	$\Gamma 1+$ (a)	$R1+$ (a)	$X1+$ $(a,0,0)$	$M1+$ $(a,0,0)$
Displacement Pattern				
Strain Vector	$(a,a,a,0,0,0)$	-	-	-
Crystal Space Group (Schönflies)	$Pm\overline{3}m$ (O_h^1)	$Fm\overline{3}m$ (O_h^5)	$P4/mmm$ (D_{4h}^1)	$P4/mmm$ (D_{4h}^1)
Local Octahedral Symmetry	O_h	O_h	D_{4h}	D_{4h}

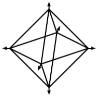
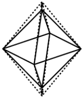
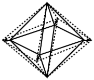
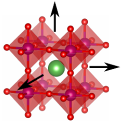
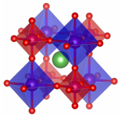
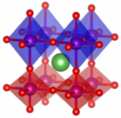
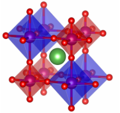
Q_1-Modes and Strains

Q_1 		Q_1^{M} 
Origin in A Ref. $Pm\bar{3}m$ B		$M4+$ $(a, 0, 0)$ $M1+$ $(a, 0, 0)$
Displacement Pattern		
Strain Vector		-
Crystal Space Group (Schönflies)		$P4/mmm$ (D_{4h}^1)
Local Octahedral Symmetry		D_{4h}

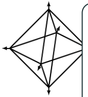
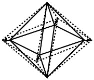
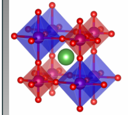


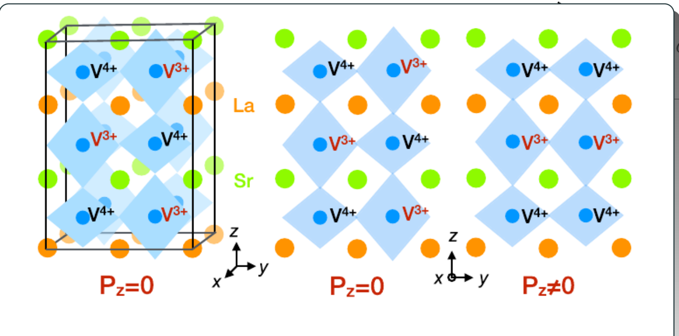
Mercy, A. *et al.*, Nat. Commun., 2017, **8**, 1677

Q_1-Modes and Strains

Q_1 	Q_1^{Γ}	$Q_1^{\mathbf{R}}$	$Q_1^{\mathbf{X}}$ 	$Q_1^{\mathbf{M}}$ 
Origin in A Ref. $Pm\overline{3}m$ B	$\Gamma1+$ (a) $\Gamma1+$ (a)	$R2-$ (a) $R1+$ (a)	$X3-$ $(a,0,0)$ $X1+$ $(a,0,0)$	$M4+$ $(a,0,0)$ $M1+$ $(a,0,0)$
Displacement Pattern				
Strain Vector	$(a,a,a,0,0,0)$	-	-	-
Crystal Space Group (Schönflies)	$Pm\overline{3}m$ (O_h^1)	$Fm\overline{3}m$ (O_h^5)	$P4/mmm$ (D_{4h}^1)	$P4/mmm$ (D_{4h}^1)
Local Octahedral Symmetry	O_h	O_h	D_{4h}	D_{4h}

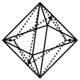
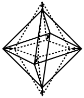
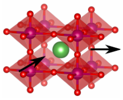
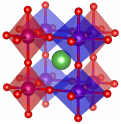
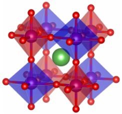
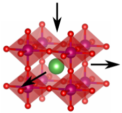
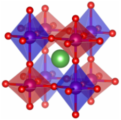
Q_1-Modes and Strains

Q_1 	Q_1^{M} 
Origin in Ref. $Pm\bar{3}m$	$M4+\ (a,0,0)$ $M1+\ (a,0,0)$
Displacement Pattern	
Strain Vector	-
Crystal Space Gr (Schönflies)	$P4/mmm$ (D_{4h}^1)
Local Octahedr Symmetry	D_{4h}

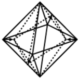
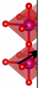
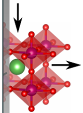
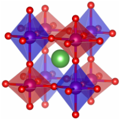


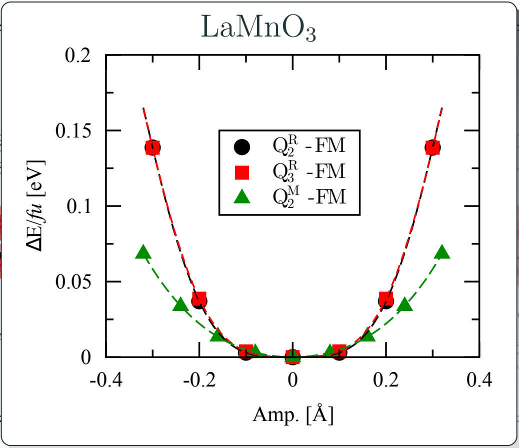
Park, S. Y. *et al.* Phys. Rev. Lett., 2017, **118**, 087602

Q_2/Q_3-Modes and Strains

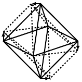
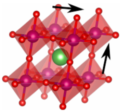
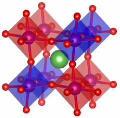
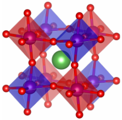
Q_2 	$Q_2^{\mathbf{\Gamma}}$	$Q_2^{\mathbf{M}}$	$Q_2^{\mathbf{R}}$	Q_3 	$Q_3^{\mathbf{\Gamma}}$	$Q_3^{\mathbf{R}}$
Origin in A	$\Gamma3+\ (0,a)$	$M3+\ (a,0,0)$	$R3-\ (0,a)$		$\Gamma3+\ (a,0)$	$R3-\ (a,0)$
Ref. $Pm\bar{3}m$ B	$\Gamma3+\ (0,a)$	$M2+\ (a,0,0)$	$R3+\ (0,a)$		$\Gamma3+\ (a,0)$	$R3+\ (a,0)$
Displacement Pattern						
Strain Vector	$(0,-a,a,0,0,0)$	-	-		$(-2a,a,a,0,0,0)$	-
Crystal Space Group (Schönflies)	$Pmmm$ (D_{2h}^1)	$P4/mbm$ (D_{4h}^5)	$I4/mcm$ (D_{4h}^{18})		$P4/mmm$ (D_{4h}^1)	$I4/mmm$ (D_{4h}^{17})
Local Octahedral Symmetry	D_{2h}	D_{2h}	D_{2h}		D_{4h}	D_{4h}

Q_2/Q_3-Modes and Strains

				$Q_3^{\mathbf{\Gamma}}$	$Q_3^{\mathbf{R}}$
Q_2 					
Origin in	A	Γ3		+ $(a, 0)$	$R3-$ $(a, 0)$
Ref. $Pm\bar{3}m$	B	Γ3		+ $(a, 0)$	$R3+$ $(a, 0)$
Displacement Pattern					
Strain Vector		$(0, -$		$a, a, 0, 0, 0)$	-
Crystal Space Group (Schönflies)		P		$/mmm$ (D_{4h}^1)	$I4/mmm$ (D_{4h}^{17})
Local Octahedral Symmetry				D_{4h}	D_{4h}



Q_4, Q_5, Q_6-Modes and Strains

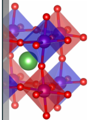
$Q_{4,5,6}$ 	$Q_4^{\mathbf{\Gamma}}$	$Q_4^{\mathbf{M}}$	$Q_4^{\mathbf{R}}$
Origin in A	$\Gamma5+$ $(a, 0, 0)$	$M1+$ $(a, 0, 0)$	$R4-$ $(a, 0, 0)$
Ref. $Pm\bar{3}m$ B	$\Gamma5+$ $(a, 0, 0)$	$M4+$ $(a, 0, 0)$	$R5+$ $(a, 0, 0)$
Displacement Pattern			
Strain Vector	$(0, 0, 0, a, 0, 0)$	-	-
Crystal Space Group (Schönflies)	$Cmmm$ (D_{2h}^{19})	$P4/mmm$ (D_{4h}^{1})	$I4/mmm$ (D_{4h}^{17})
Local Octahedral Symmetry	D_{2h}	D_{2h}	D_{2h}

Q_4, Q_5, Q_6-Modes and Strains

$Q_{4,5,6}$  $Q_4^{\mathbf{R}}$

Origin ... $(a, 0, 0)$

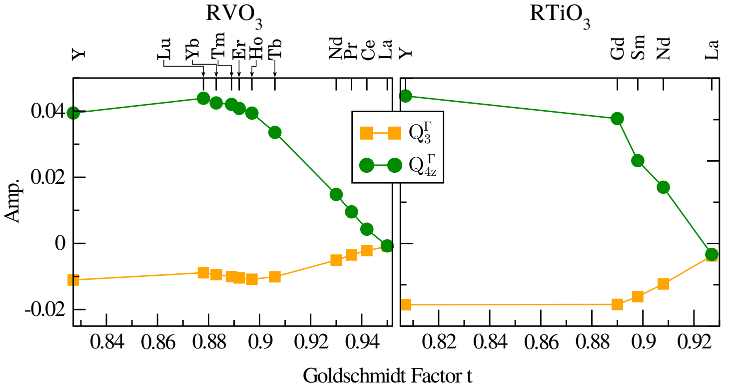
Ref. Pn ... $(a, 0, 0)$

Displac... Patt... 

Strain V... -

Crystal Spa... (Schön... ... $4/mmm$ (D_{4h}^{17})

Local Oc... Symm... ... D_{2h}



Martínez-Lope, M. J. *et al.* Inorg. Chem., 2008, **47**, 2634-264

Komarek, A. C. *et al.* Phys. Rev. B, 2007, **75**, 224402

$LaMnO_3$

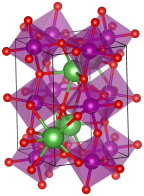
Bulk

JTD In $LaMnO_3$

GS

$Pnma\ a^- a^- c^+$

+ JTD

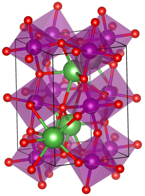


JTD In $LaMnO_3$

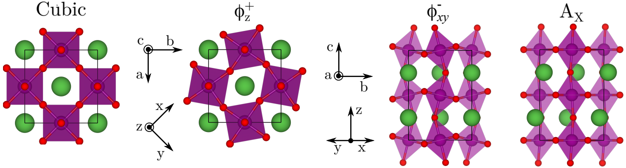
GS

$Pnma\ a^- a^- c^+$

+ JTD



O-Phase $750K < T < 1200K$ Metallic

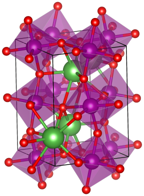


JTD In $LaMnO_3$

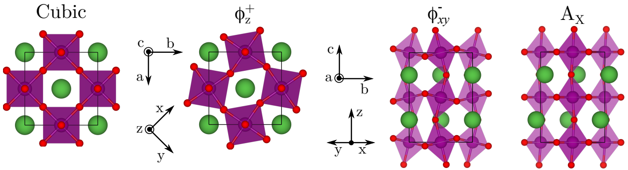
GS

$Pnma\ a^- a^- c^+$

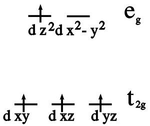
+ JTD



O-Phase $750K < T < 1200K$ Metallic



$Mn^{3+} = d^4$

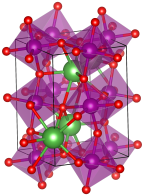


JTD In $LaMnO_3$

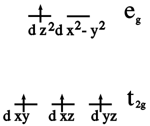
GS

$Pnma\ a^- a^- c^+$

+ JTD

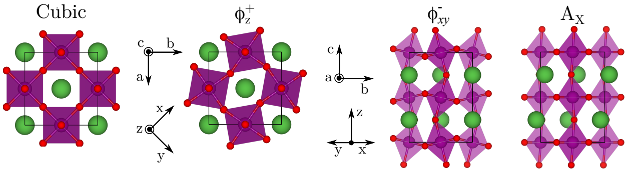


$Mn^{3+} = d^4$

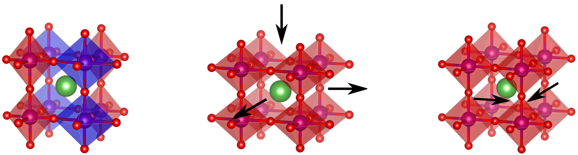


$\rightarrow$

O-Phase $750K < T < 1200K$ Metallic



O'-Phase $T < T_{JT} = 750K$ Ins. - AFM-A T < 140K

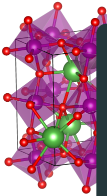


JTD In $LaMnO_3$

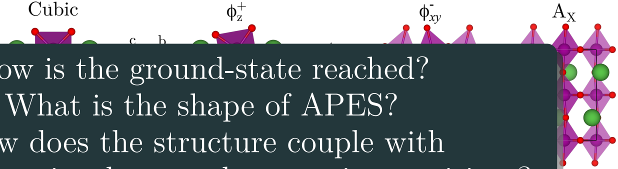
GS

Pnma $a^- a^- c^+$

+ JTD



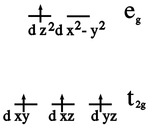
O-Phase $750K < T < 1200K$ Metallic



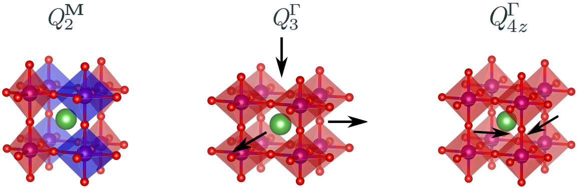
How is the ground-state reached?
What is the shape of APES?
How does the structure couple with
the metal to insulator and magnetic transition ?
Let's ask DFT!

O'-Phase $T < T_{JT} = 750K$ Ins. - AFM-A $T < 140K$

$Mn^{3+} = d^4$



→

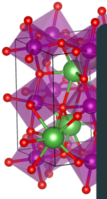


JTD In $LaMnO_3$

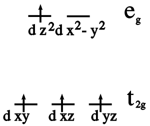
GS

$Pnma\ a^-a^-c^+$

+ JTD

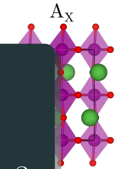


$\mathbf{Mn^{3+} = d^4}$



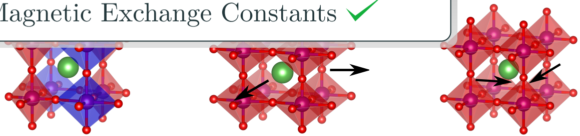
the r… …ion ?

…tallic



…A T < 140K

Q^{Γ}_{4z}



K-Mesh 14x14x14 - $E_{cut} = 600eV$

E_{xc} = PBEsol + (U|J)

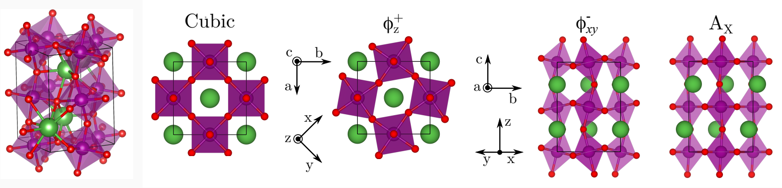
U=5.5 eV J=1.5 eV

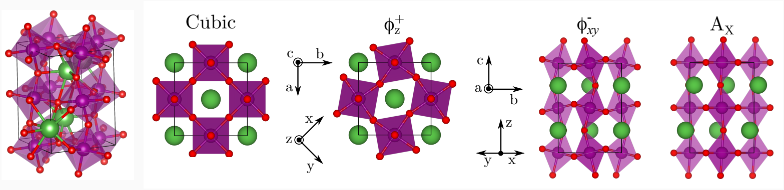
Ground State Structure ✓

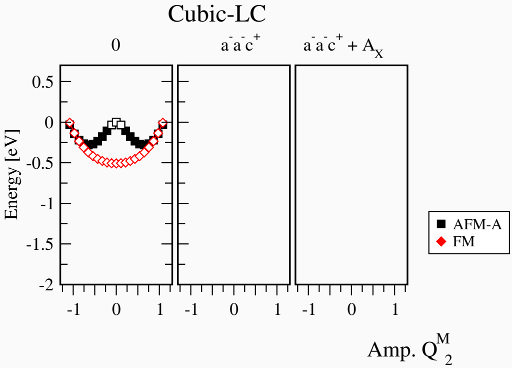
Band Gap (1.1 eV - Exp 1.1 - 1.9 eV) ✓

Anistropy of Dielectric Tensor ✓

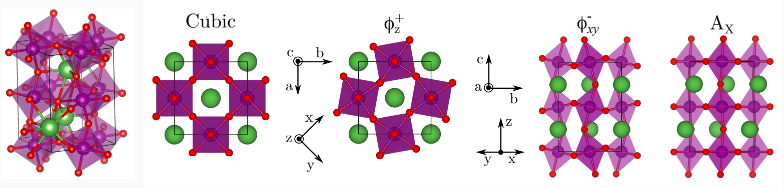
Magnetic Exchange Constants ✓

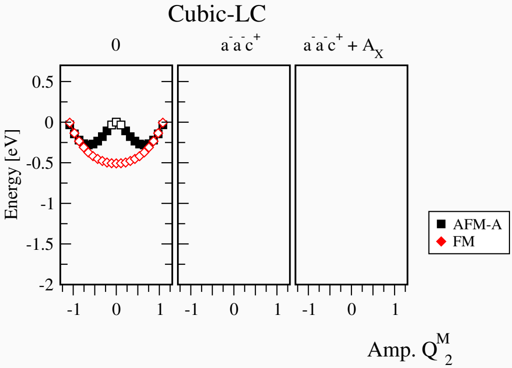

Cubic
c
b
a
x
z
y
ϕ_z^+
c
a
b
z
y
x
ϕ_{xy}^-
A_X





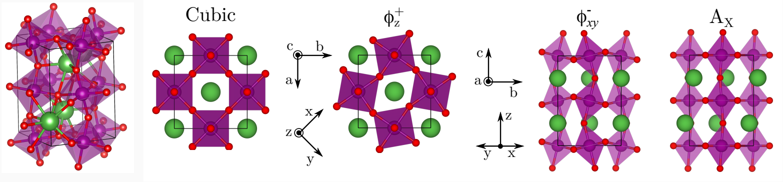
$$F \propto \alpha_{el} Q_2^M + \beta_1 {Q_2^M}^2$$

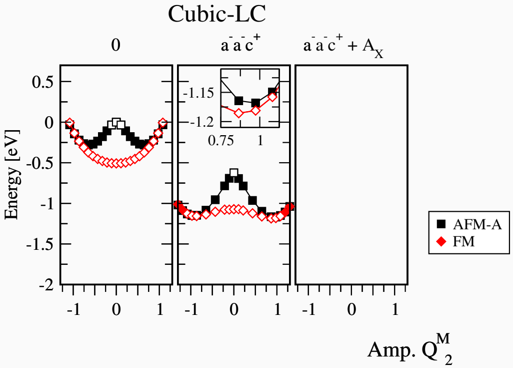




$$F \propto \alpha_{el} Q_2^M + \beta_1 Q_2^{M^2}$$

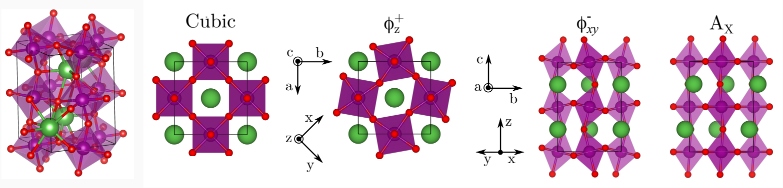
$$\alpha_{el} = \left\langle \Psi_i^0 \middle| \frac{\partial H_0}{\partial Q_2^M} \middle| \Psi_j^0 \right\rangle \Rightarrow \alpha_{el}(MO)$$

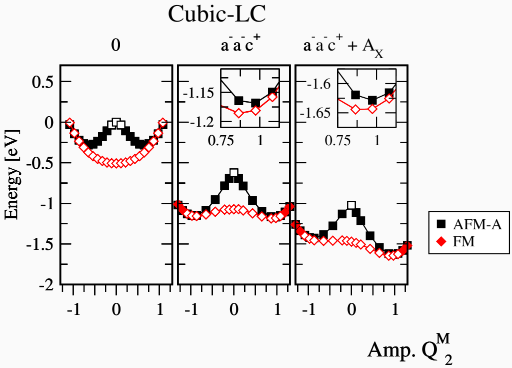




$$F \propto \alpha_{el} Q_2^M + \beta_1 Q_2^{M^2} + \beta_2 \phi^2 Q_2^{M^2}$$

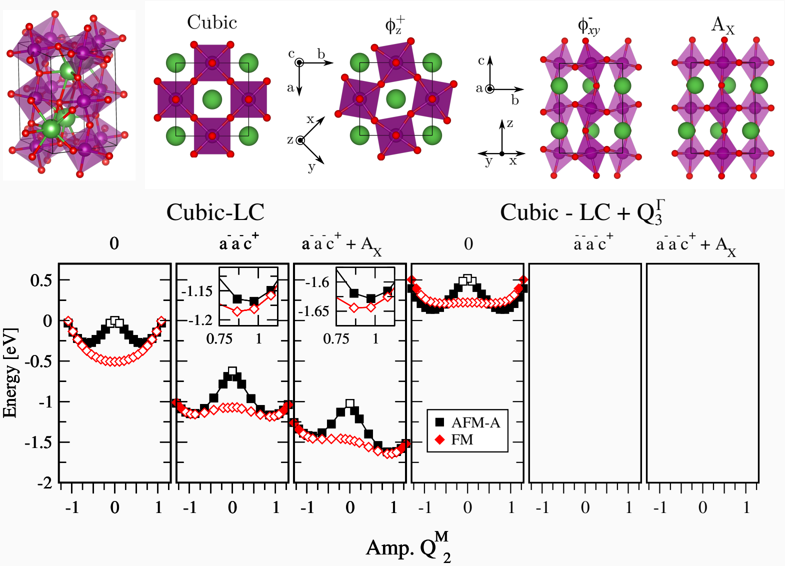
$$\alpha_{el} = \left\langle \Psi_i^0 \middle| \frac{\partial H_0}{\partial Q_2^M} \middle| \Psi_j^0 \right\rangle \Rightarrow \alpha_{el}(MO, \{\mathbf{R}\})$$





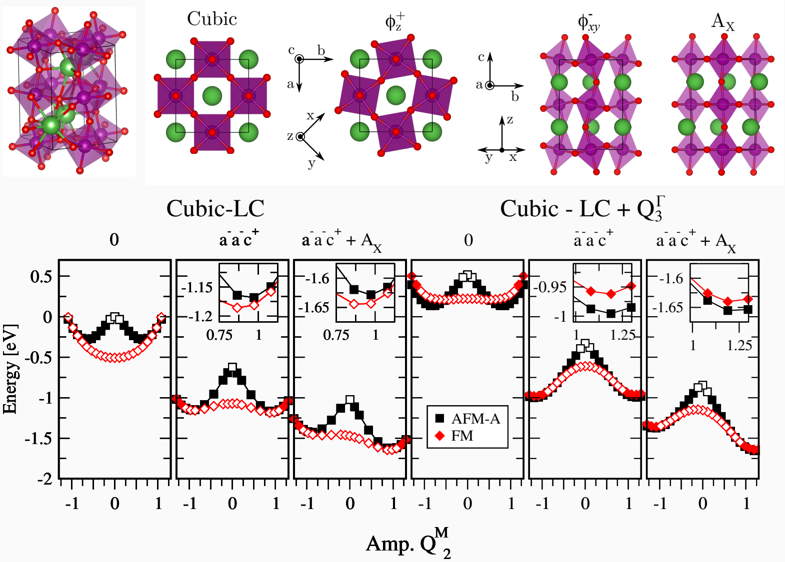
$$F \propto \alpha_{el} Q_2^M + \beta_1 Q_2^{M^2} + \beta_2 \phi^2 Q_2^{M^2} + \gamma_1 A P_{xy} \phi^- Q_2^M$$

$$\alpha_{el} = \left\langle \Psi_i^0 \middle| \frac{\partial H_0}{\partial Q_2^M} \middle| \Psi_j^0 \right\rangle \Rightarrow \alpha_{el}(MO, \{\mathbf{R}\})$$



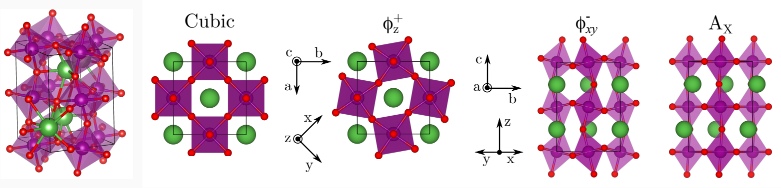
$$F \propto \alpha_{el} Q_2^M + \beta_1 Q_2^{M^2} + \beta_2 \phi^2 Q_2^{M^2} + \gamma_1 A P_{xy} \phi^- Q_2^M + \beta_3 Q_3^\Gamma Q_2^{M^2} + \beta_4 Q_3^{\Gamma^2} Q_2^{M^2}$$

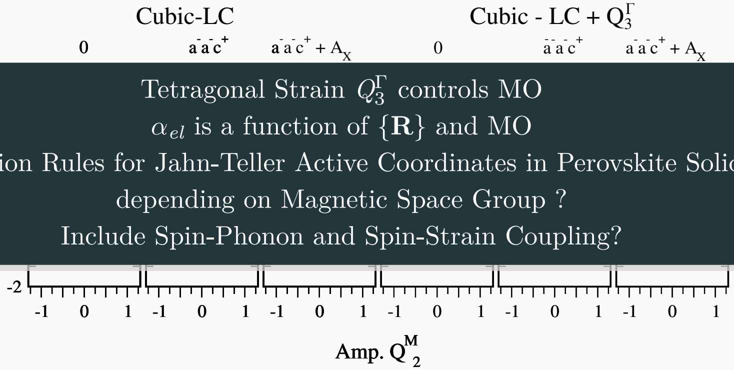
$$\alpha_{el} = \left\langle \Psi_i^0 \left| \frac{\partial H_0}{\partial Q_2^M} \right| \Psi_j^0 \right\rangle \Rightarrow \alpha_{el}(MO, \{\mathbf{R}\})$$



$$F \propto \alpha_{el} Q_2^M + \beta_1 Q_2^{M^2} + \beta_2 \phi^2 Q_2^{M^2} + \gamma_1 A P_{xy} \phi^- Q_2^M + \beta_3 Q_3^\Gamma Q_2^{M^2} + \beta_4 Q_3^{\Gamma^2} Q_2^{M^2}$$

$$\alpha_{el} = \left\langle \Psi_i^0 \middle| \frac{\partial H_0}{\partial Q_2^M} \middle| \Psi_j^0 \right\rangle \Rightarrow \alpha_{el}(MO, \{\mathbf{R}\})$$





Tetragonal Strain Q_3^Γ controls MO

α_{el} is a function of $\{\mathbf{R}\}$ and MO

Selection Rules for Jahn-Teller Active Coordinates in Perovskite Solids depending on Magnetic Space Group ?

Include Spin-Phonon and Spin-Strain Coupling?

$$F \propto \alpha_{el} Q_2^M + \beta_1 Q_2^{M^2} + \beta_2 \phi^2 Q_2^{M^2} + \gamma_1 A P_{xy} \phi^- Q_2^M + \beta_3 Q_3^\Gamma Q_2^{M^2} + \beta_4 Q_3^{\Gamma^2} Q_2^{M^2}$$

$$\alpha_{el} = \left\langle \Psi_i^0 \middle| \frac{\partial H_0}{\partial Q_2^M} \middle| \Psi_j^0 \right\rangle \Rightarrow \alpha_{el}(MO, \{\mathbf{R}\})$$

$LaMnO_3$

Epitaxial Thin Films

Ferromagnetic $LaMnO_3$ on $SrTiO_3$

REPORTS

MAGNETISM

Imaging and control of ferromagnetism in $LaMnO_3/SrTiO_3$ heterostructures

X. Renshaw Wang,[1*†‡] C. J. Li,[2,3†] W. M. Lü,[2] T. R. Paudel,[4] D. P. Leusink,[1] M. Hoek,[1] N. Poccia,[1] A. Vailionis,[5] T. Venkatesan,[2,3,6,7*] J. M. D. Coey,[2,8] E. Y. Tsymbal,[4] Ariando,[2,6] H. Hilgenkamp[1]

Ferromagnetic $LaMnO_3$ on $SrTiO_3$

REPORTS

CRYSTAL GROWTH & DESIGN

Article

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Strain-Engineered Ferromagnetism in $LaMnO_3$ Thin Films

Jaume Roqueta,[†] Alberto Pomar,[*,‡] Lluis Balcells,[‡] Carlos Frontera,[‡] Sergio Valencia,[∥] Radu Abrudan,[∥,⊥] Bernat Bozzo,[‡] Zorica Konstantinović,[‡,§] José Santiso,[†] and Benjamín Martínez[‡]

[†]Institut Català de Nanociència i Nanotecnologia, ICN2 (CSIC-ICN), Campus de la UAB, 08193 Bellaterra, Spain

[‡]Instituto de Ciencia de Materiales de Barcelona-CSIC, Campus de la UAB, 08193 Bellaterra, Spain

[§]Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

[∥]Helmholtz-Zentrum-Berlin für Materialien und Energie, Albert-Einstein Strasse 15, D-12489 Berlin, Germany

[⊥]Institut für Experimentalphysik/Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

Ferromagnetic $LaMnO_3$ on $SrTiO_3$

REPORTS

CRYSTAL GROWTH & DESIGN

Article

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ACS APPLIED MATERIALS & INTERFACES

Research Article

www.acsami.org

Room-Temperature Ferromagnetism in Thin Films of $LaMnO_3$ Deposited by a Chemical Method Over Large Areas

José Manuel Vila-Fungueiriño,[†] Beatriz Rivas-Murias,[†] Benito Rodríguez-González,[‡] O. Txoperena,[§] D. Ciudad,[§] Luis E. Hueso,[§] Massimo Lazzari,[†] and Francisco Rivadulla*,[†]

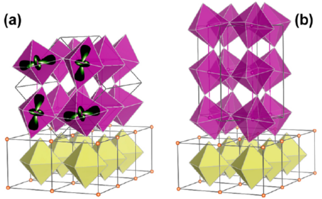
[†]Centro de Investigación en Química Biológica y Materiales Moleculares (CIQUS), Universidad de Santiago de Compostela, 15782 Santiago de Compostela, Spain

[‡]Departamento de Química Física, Universidad de Vigo, 36310 Vigo, Spain

[§]CIC-nanoGUNE and IKERBASQUE, Basque Foundation for Science, 20018 San Sebastian, Spain

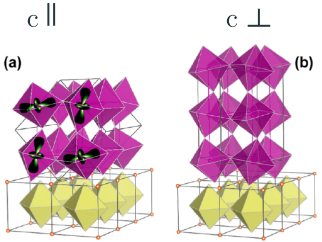
Ferromagnetic $LaMnO_3$ on $SrTiO_3$

c ∥ c ⊥

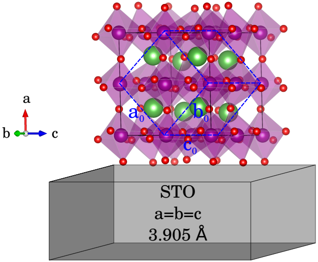


Roqueta J.,*et al.* Cryst. Growth Des. **15.11** (2015)

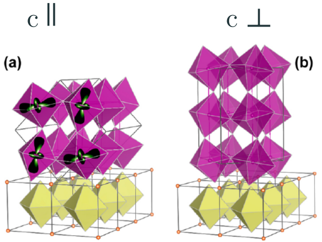
Ferromagnetic $LaMnO_3$ on $SrTiO_3$



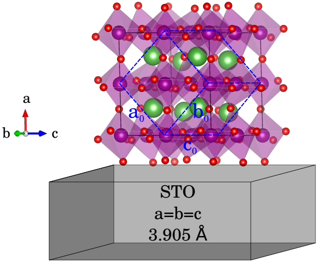
Roqueta J., *et al.* Cryst. Growth Des. **15.11** (2015)



Ferromagnetic $LaMnO_3$ on $SrTiO_3$

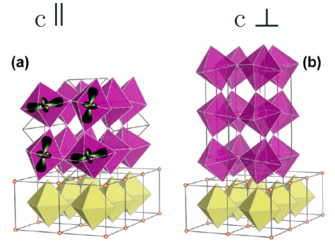


Roqueta J., *et al.* Cryst. Growth Des. **15.11** (2015)

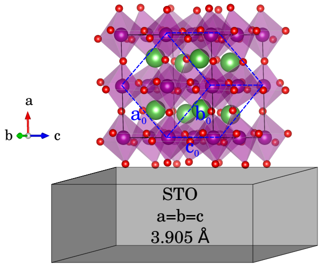


	LMO-STO	LMO-Bulk
	P-1	*Pnma*
	FM	AFM-A
Q_3^{Γ}	-0.005	-0.04
Q_{4z}^{Γ}	-0.018	-0.036
Q_2^M (Å)	0.117	0.19
Q_3^R (Å)	0.077	-
ϕ_z^+ (Å)	0.44	0.49
ϕ_{xy}^- (Å)	0.62	0.65
A_X (Å)	0.26	0.33
Band Gap (eV)	0.49	1.15

Ferromagnetic $LaMnO_3$ on $SrTiO_3$



Roqueta J., *et al.* Cryst. Growth Des. **15.11** (2015)



	LMO-STO	LMO-Bulk
	P-1	*Pnma*
	FM	AFM-A
Q_3^Γ	-0.005	-0.04
Q_{4z}^Γ	-0.018	-0.036
Q_2^M (Å)	0.117	0.19
Q_3^R (Å)	0.077	-
ϕ_z^+ (Å)	0.44	0.49
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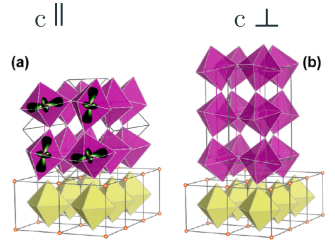
Ferromagnetic $LaMnO_3$ on $SrTiO_3$



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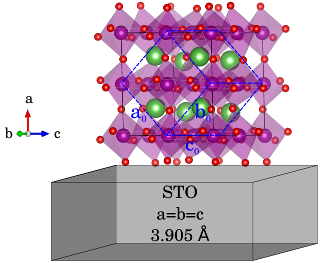

	LMO-STO	LMO-Bulk
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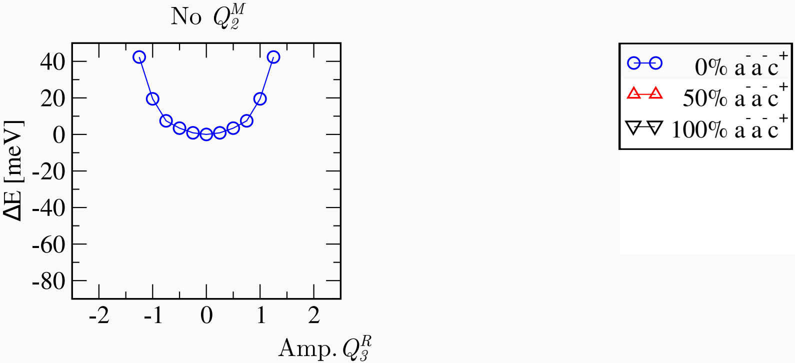
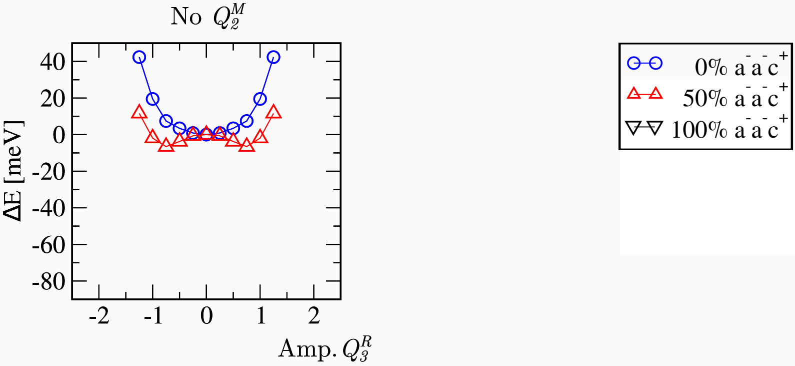
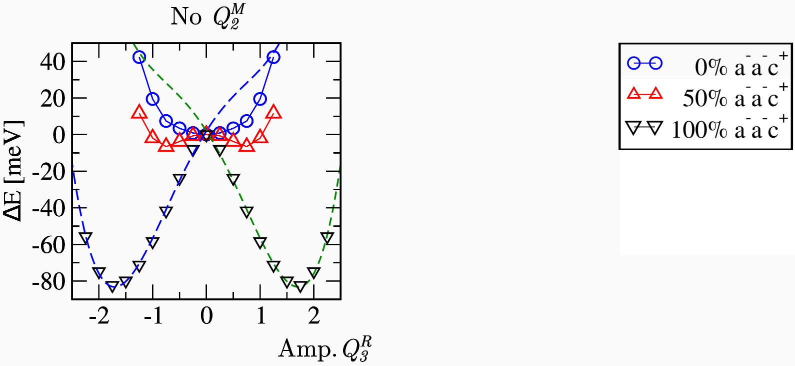
Q_3^R JTD



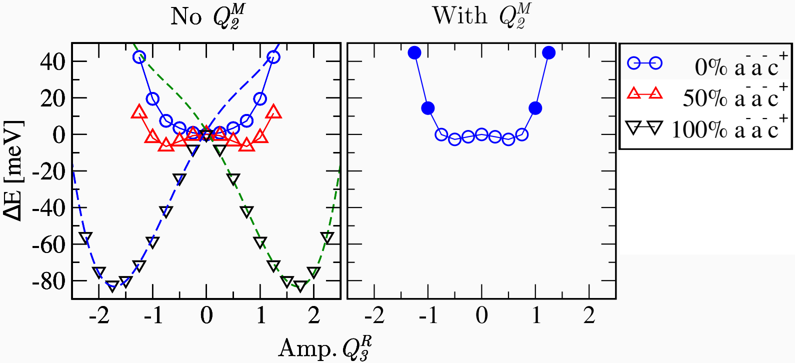
Q_3^R JTD



Q_3^R JTD

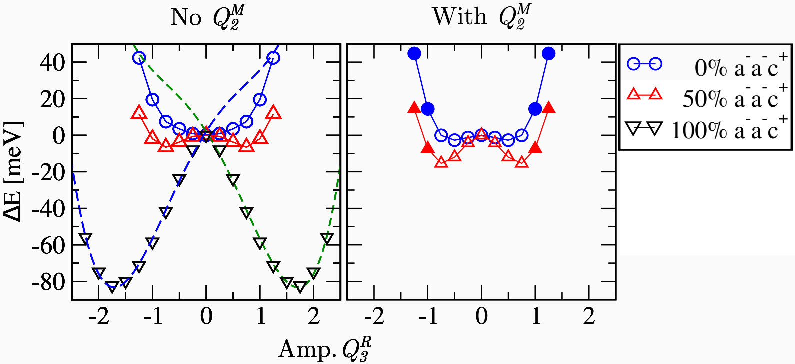


Q_3^R JTD



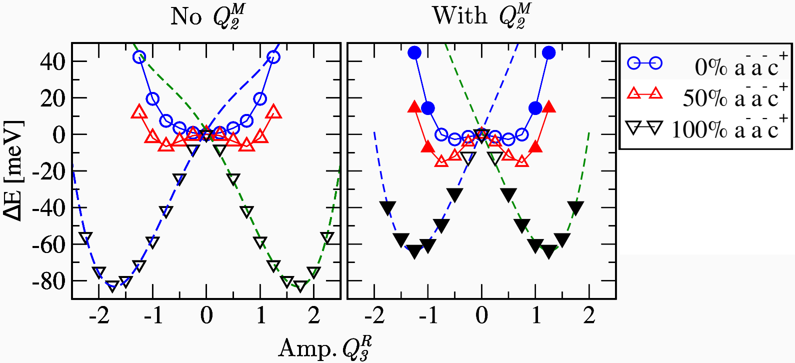
No Q_2^M
With Q_2^M
0% a⁻a⁻c⁺
50% a⁻a⁻c⁺
100% a⁻a⁻c⁺
ΔE [meV]
40
20
0
-20
-40
-60
-80
-2
-1
0
1
2
Amp. Q_3^R

Q_3^R JTD

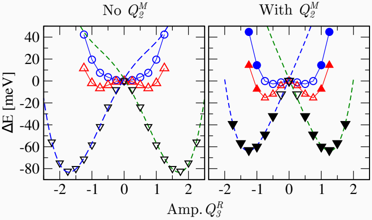


No Q_2^M
With Q_2^M
ΔE [meV]
40
20
0
-20
-40
-60
-80
-2
-1
0
1
2
Amp. Q_3^R
0% a⁻a⁻c⁺
50% a⁻a⁻c⁺
100% a⁻a⁻c⁺

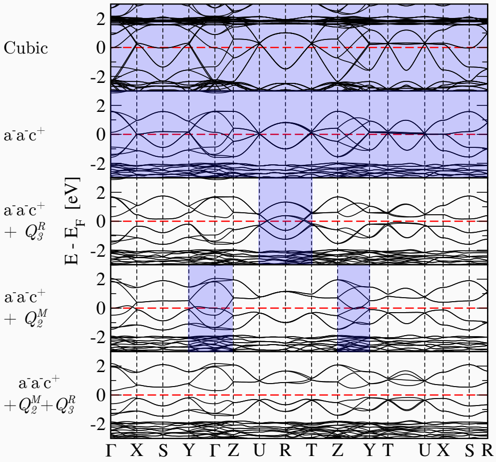
Q_3^R JTD



Q_3^R JTD

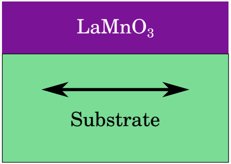


No Q_2^M
With Q_2^M
ΔE [meV]
40
20
0
-20
-40
-60
-80
-2
-1
0
1
2
Amp. Q_3^R

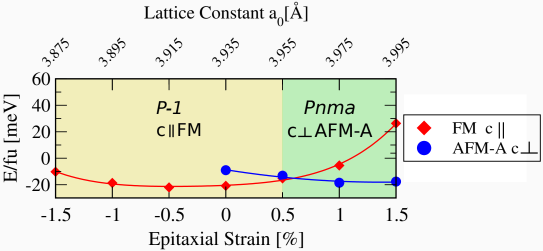


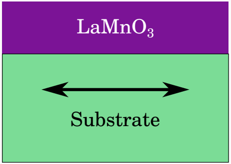
Cubic
a⁻a⁻c⁺
a⁻a⁻c⁺ + Q_3^R
a⁻a⁻c⁺ + Q_2^M
a⁻a⁻c⁺ + Q_2^M + Q_3^R
E - E$_F$ [eV]
2
0
-2
Γ X S Y Γ Z U R T Z Y T U X S R

Strain Engineering in $LaMnO_3$



Strain Engineering in $LaMnO_3$





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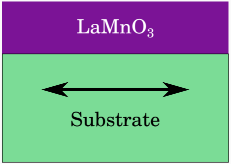

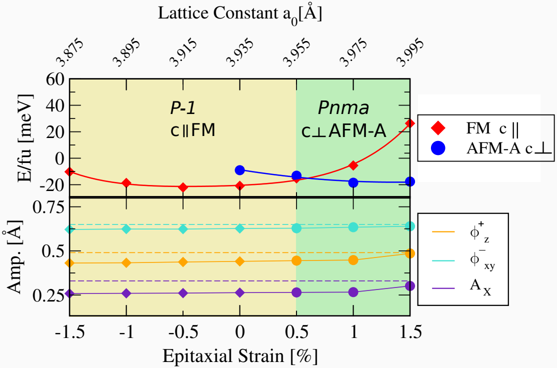

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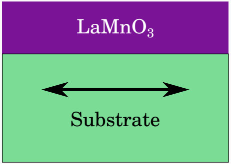
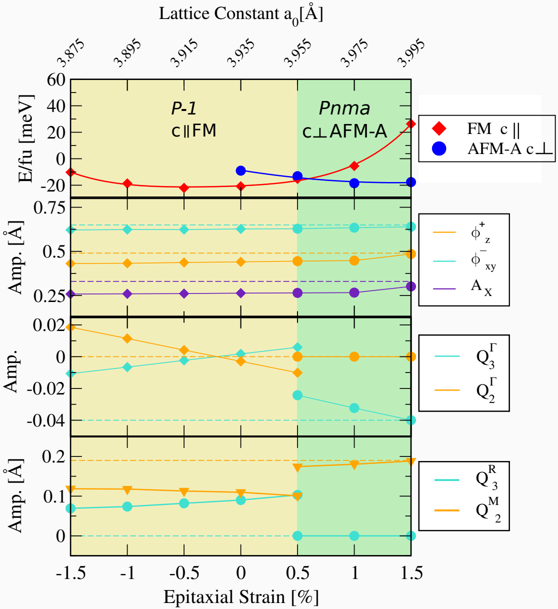
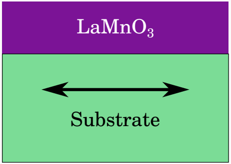
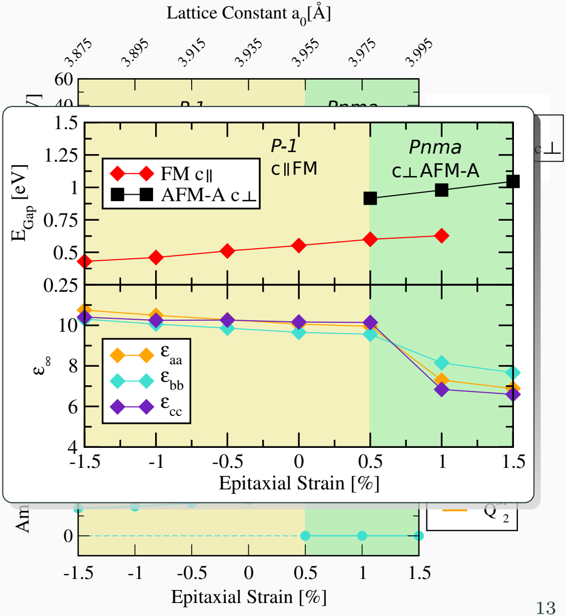




Strain Engineering in $LaMnO_3$





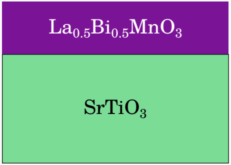
An Approach to a Ferromagnetic/Ferroelectric Multiferroic $RMnO_3$ Compound

$La_{0.5}Bi_{0.5}MnO_3$ Solid Solution on $SrTiO_3$

Break The Inversion Symmetry Through Cationic Order!

$La_{0.5}Bi_{0.5}MnO_3$ Solid Solution on $SrTiO_3$

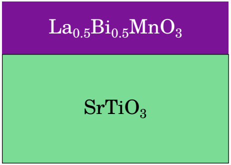
Break The Inversion Symmetry Through Cationic Order!



Cation Order	$\Delta E/fu(meV)$	MO	Space Group	BG (eV)
Layered $\parallel$	-	FM	*P-1*	-
Layered $\perp$	-5	FM	*P1* ✓	-
Chains	-3	FM	*P-1*	-
Rock-Salt	-10	FM	*P1* ✓	0.38

$La_{0.5}Bi_{0.5}MnO_3$ Solid Solution on $SrTiO_3$

Break The Inversion Symmetry Through Cationic Order!

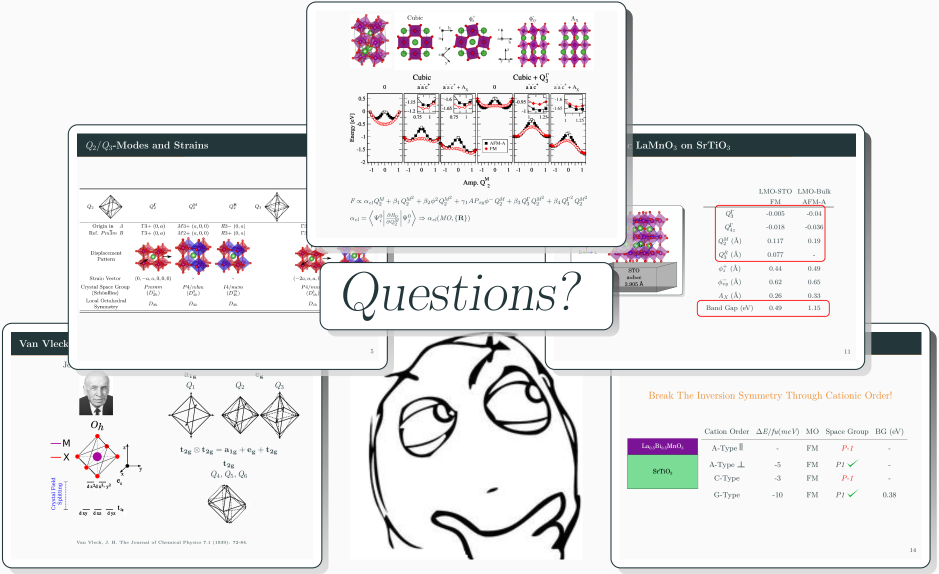


Cation Order	$\Delta E/fu(meV)$	MO	Space Group	BG (eV)
Layered ∥	-	FM	*P-1*	-
Layered ⊥	-5	FM	*P1* ✓	-
Chains	-3	FM	*P-1*	-
Rock-Salt	-10	FM	*P1* ✓	0.38

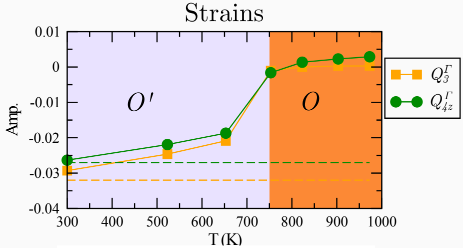
Conclusions

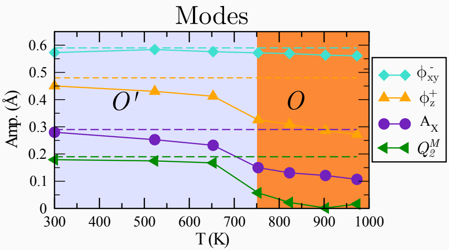
- Q_i^q a Clear and Revised Notation for Cooperative Jahn-Teller Distortions in Perovskites
- Decomposition of Distorded Perovskite Structures into orthonormal Modes and Strains Allows for Profound Studies of Structural-Electronic Interactions in Perovskite Crystal (*ISODISTORT*: http://stokes.byu.edu/iso/isodistort.php &/or *AMPLIMODES*: http://www.cryst.ehu.es/cryst/amplimodes.html)
- Study of the APES With Ab-Inito Methods Show That The Magnetic AFM-A to FM Transition is Controlled by Tetragonal Strain Q_3^Γ
- A First-Order Jahn-Teller Effect Takes Place Only in Specific Magnetic Orderings. Do we Need a Revised Jahn-Teller Theorem for Magnetic Space Groups in Solids ?
- The Characterization of Strain/Lattice/Electronic Interplays Permits to Derive New Design-Ideas for Materials with Remarkable Combination of Properties

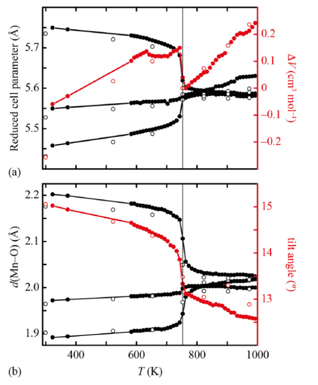
Thank you for your attention!



Modes and Strains under Temperature

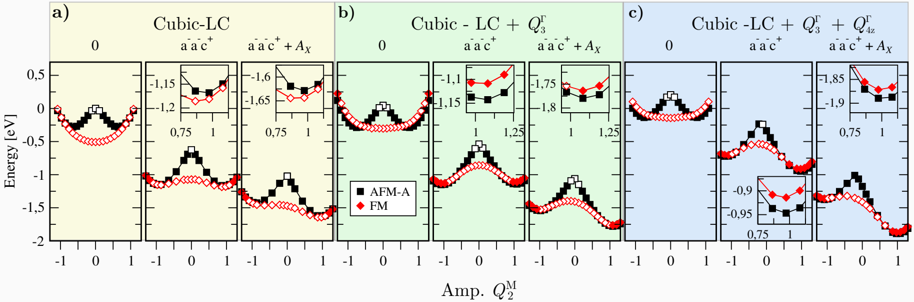




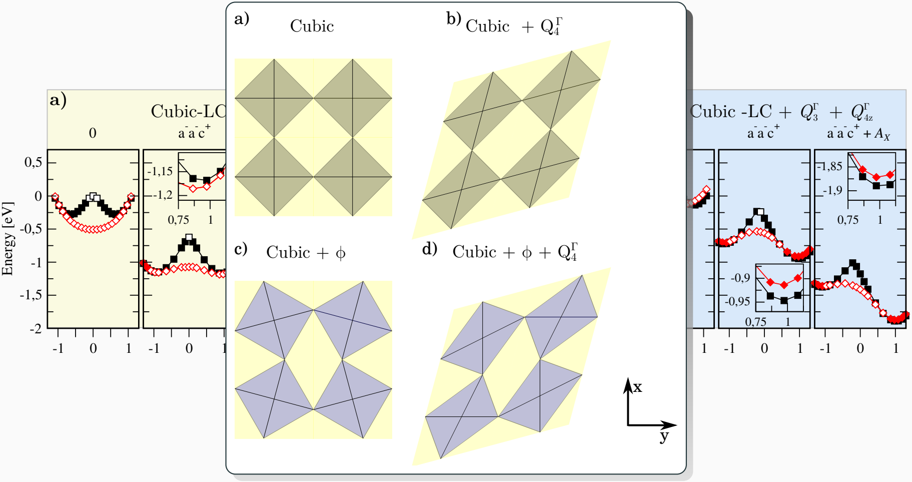


Thygesen, P. M. M. *et al.* Phys. Rev. B, 2017, **95**, 174107

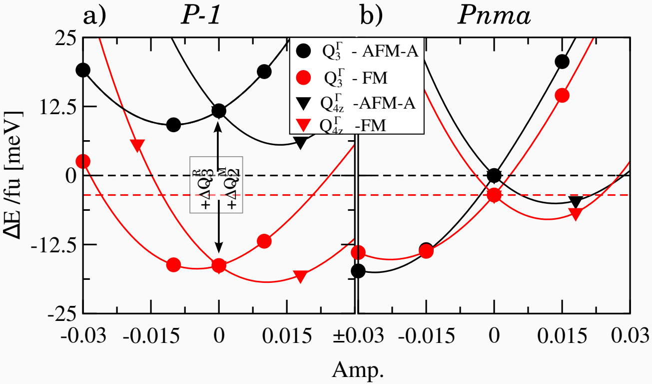
Full Potential Energy Surface



Full Potential Energy Surface

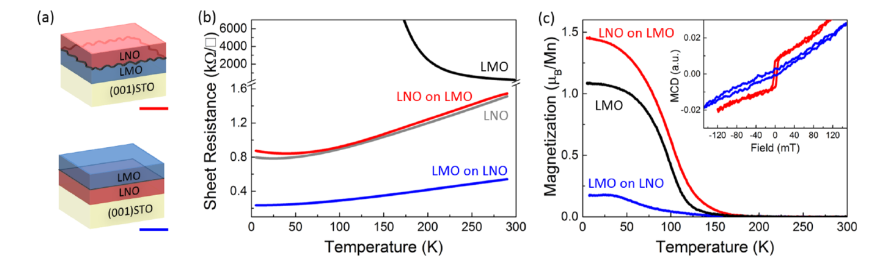


Strain APES



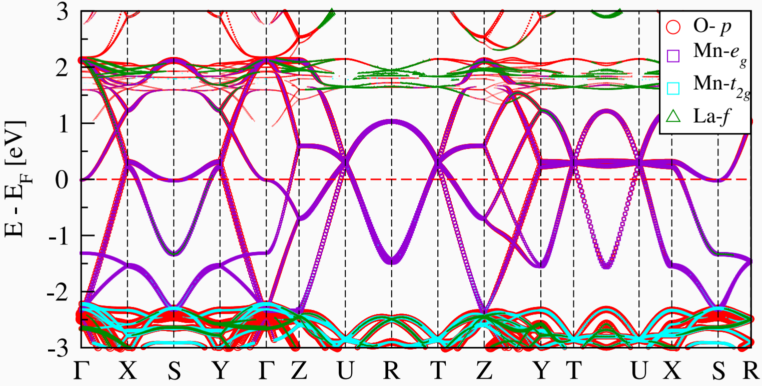
Phase	A_X[Å]	ϕ_z^+[Å]	ϕ_{xy}^-[Å]	Q_2^M[Å]	Q_3^{Γ}[Å]	E/fu[eV]
P-1	0.20	0.40	0.64	0.11	0.09	-31.744
Pnma	0.20	0.40	0.64	0.17	0	-31.728

$LaMnO_3$ $LaNiO_3$ Bilayers on $SrTiO_3$



Gibert, M., Nano Letters, 2015, **15**, 7355-736

Projected Band Structure



Influence of U|J Parameters