Canonical Jahn-Teller Distortion Notations

Understanding Structural-Electronic Interplays in $\mathbf{e_g^1}$ Perovskites

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

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16th - 19th October 2019

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

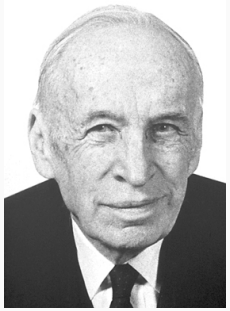
Outline

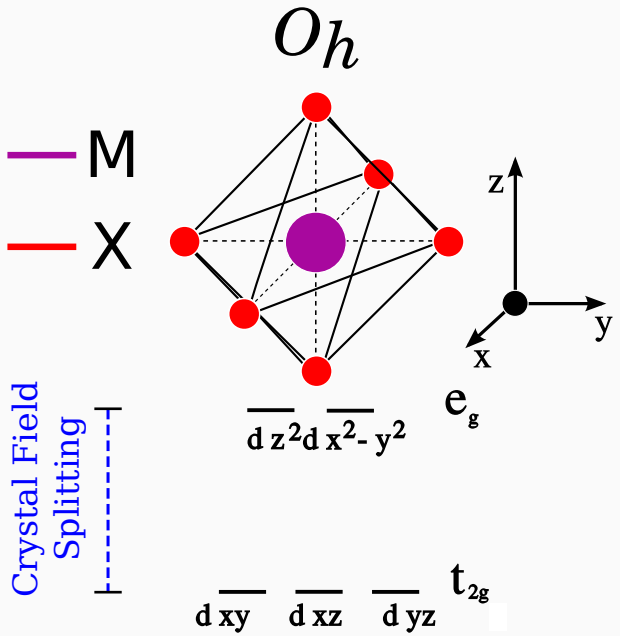
- Canonical Jahn-Teller Distortion Notations
- Application I: Bulk Ground State of $LaMnO_3$
- Application II: [001] Epitaxial Strain Phase Diagram of $CaFeO_3$
- Application III: [001] vs [111] Epitaxial Strain in $NdNiO_3$

Canonical Jahn-Teller Distortion Notations

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.

Van Vleck: The octahedral Complex MX_6

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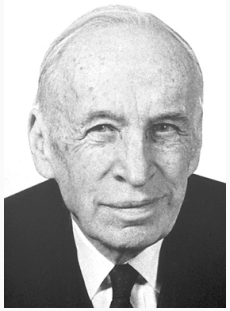
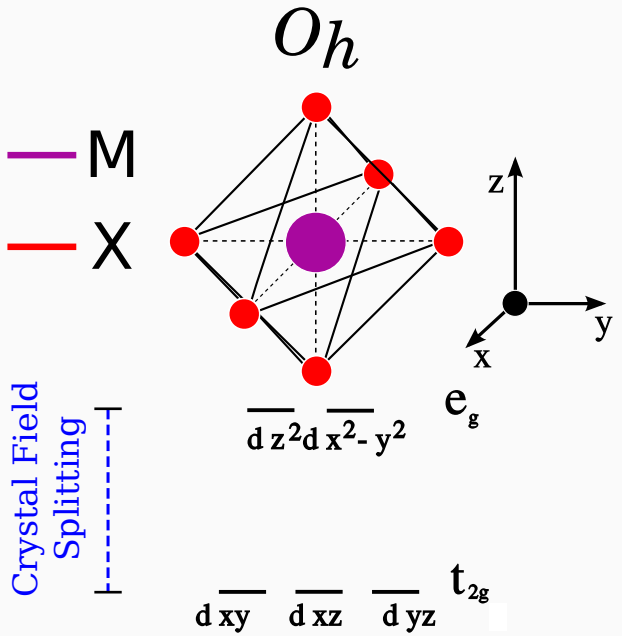
$$\mathbf{e_g} \otimes \mathbf{e_g} = \mathbf{a_{1g}} + \mathbf{e_g}$$





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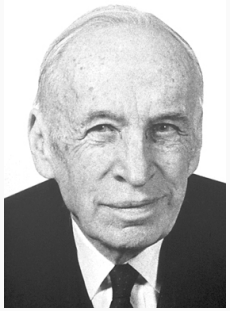
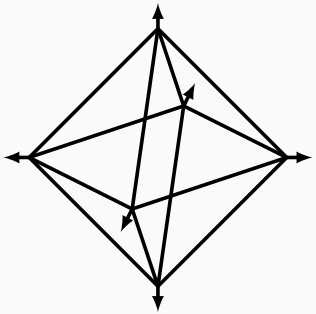


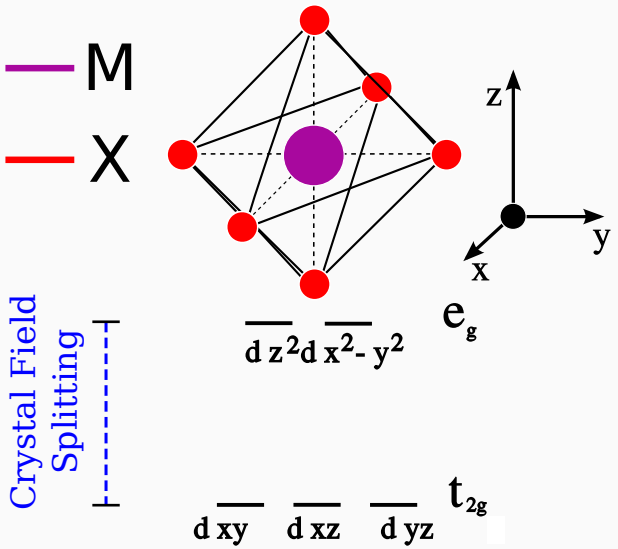
$$\mathbf{e_g} \otimes \mathbf{e_g} = \mathbf{a_{1g}} + \mathbf{e_g}$$

$\mathbf{a_{1g}}$

Q_1



O_h



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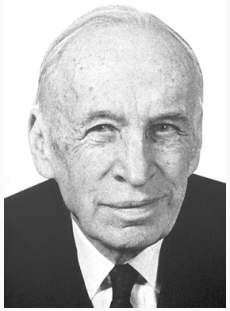

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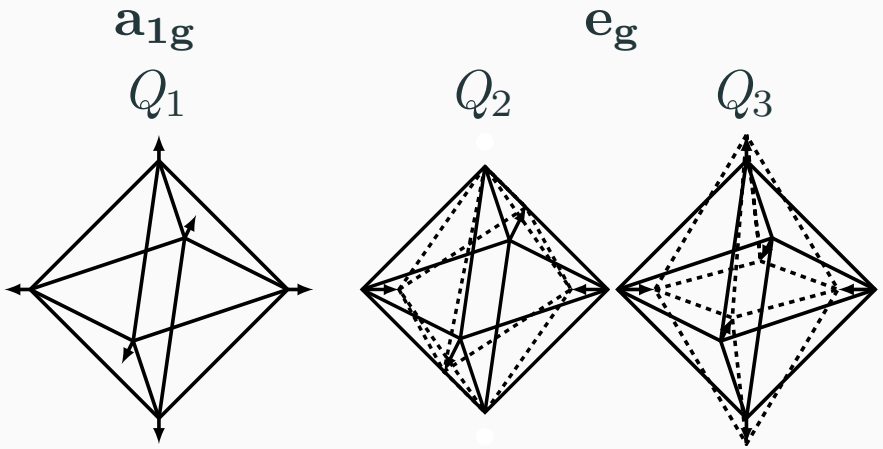

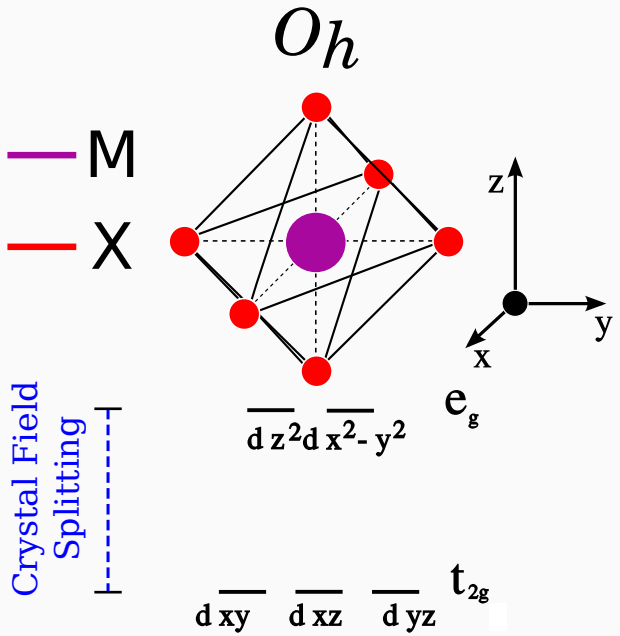

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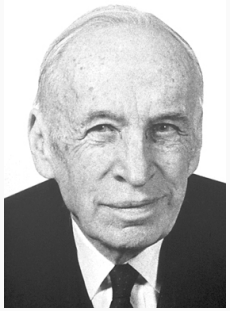
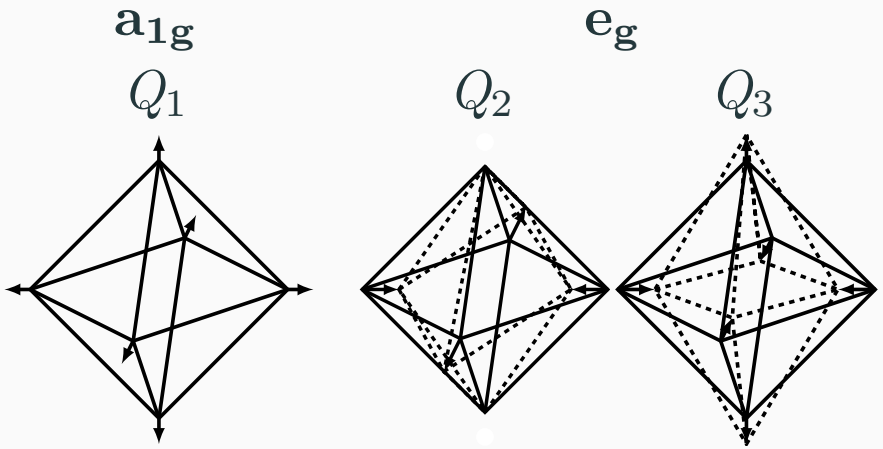
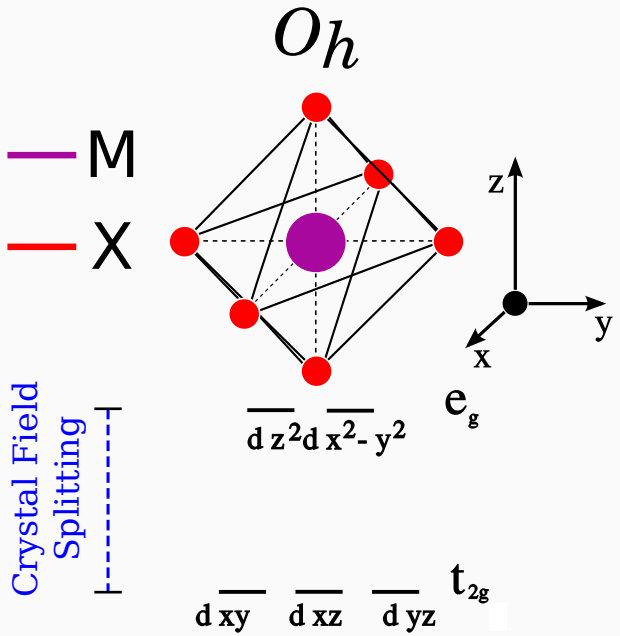


$$\mathbf{e_g} \otimes \mathbf{e_g} = \mathbf{a_{1g}} + \mathbf{e_g}$$



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



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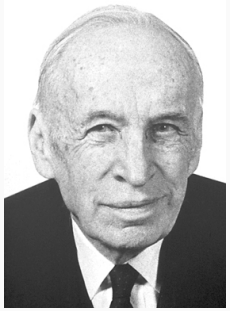
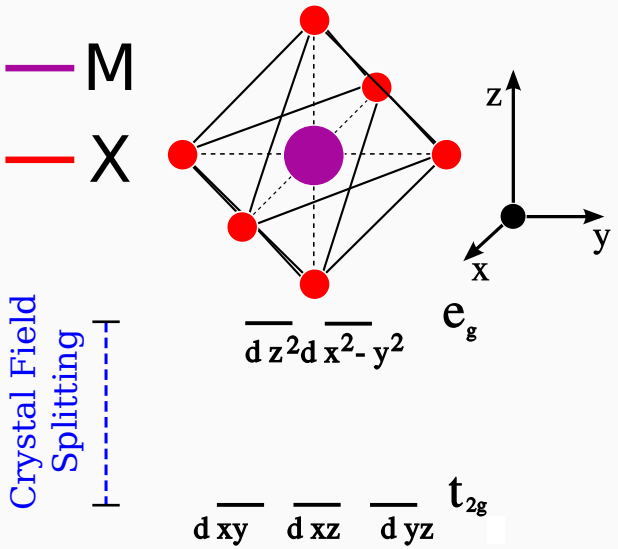


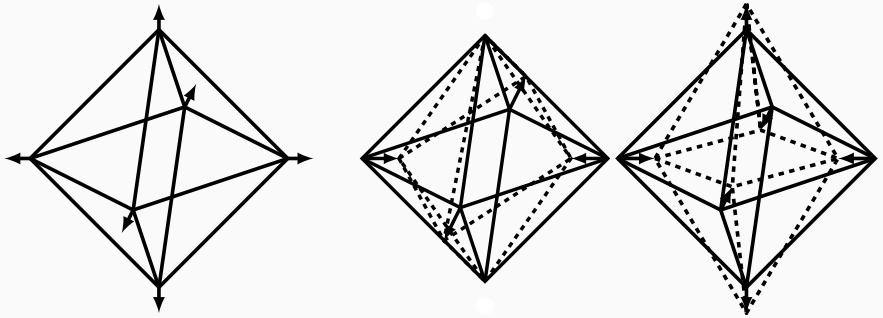
O_h



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

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

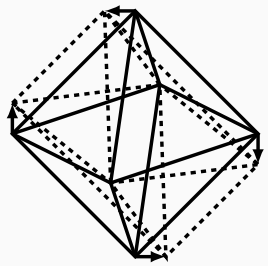
Q_1 Q_2 Q_3



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

$\mathbf{t_{2g}}$

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_θ, Q_ϵ

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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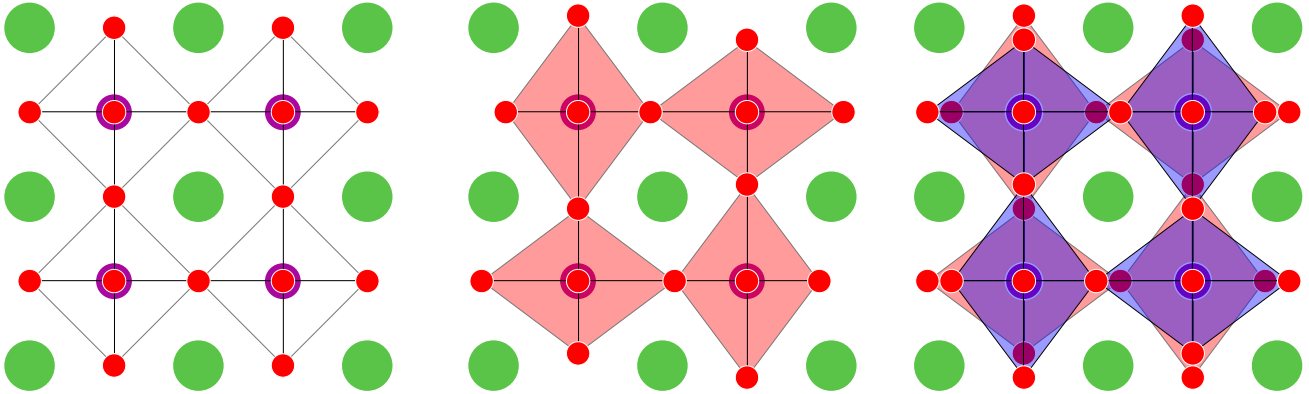
Chemists

Perovskite Structure



Same Individual Distortion

Through Different Cooperative Arrangements

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

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

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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 Canonical Notation!

$$Q_{i\alpha}^{\vec{q}}$$

i = Vlecks Numbering	$\vec{q}$ = q-vector in Cubic BZ
α = orientation (x,y,z)	$Q_i \cdot e^{iq\vec{R}}$
1	$\Gamma = (0,0,0) = Strain$
2	$X = (\frac{1}{2},0,0)$
3	$M = (\frac{1}{2},\frac{1}{2},0)$
4	$R = (\frac{1}{2},\frac{1}{2},\frac{1}{2})$

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

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

Schmitt, M. M., et al, arXiv:1909.06287 (2019)

Vaughn, S.; Bristowe, N. C. & Ghosez, P. Phys. Rev. Lett., 2016, **116**, 057602

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

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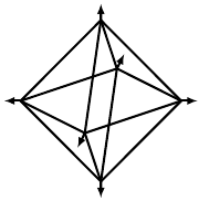
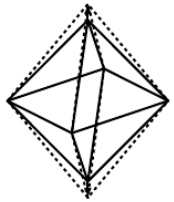
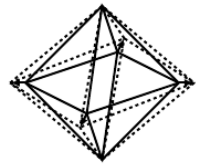
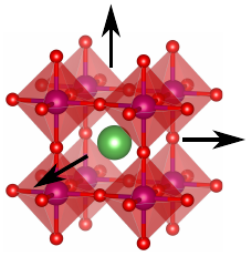
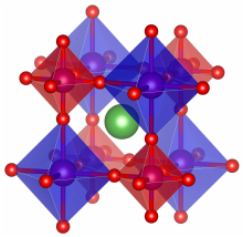
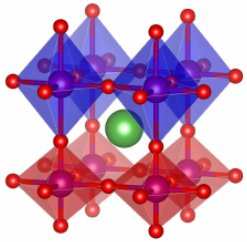
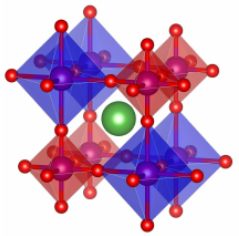
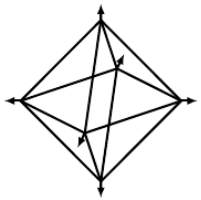
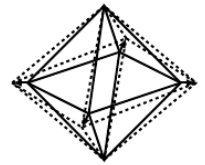
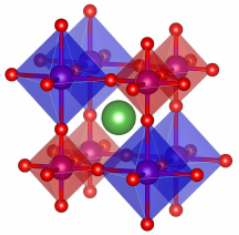
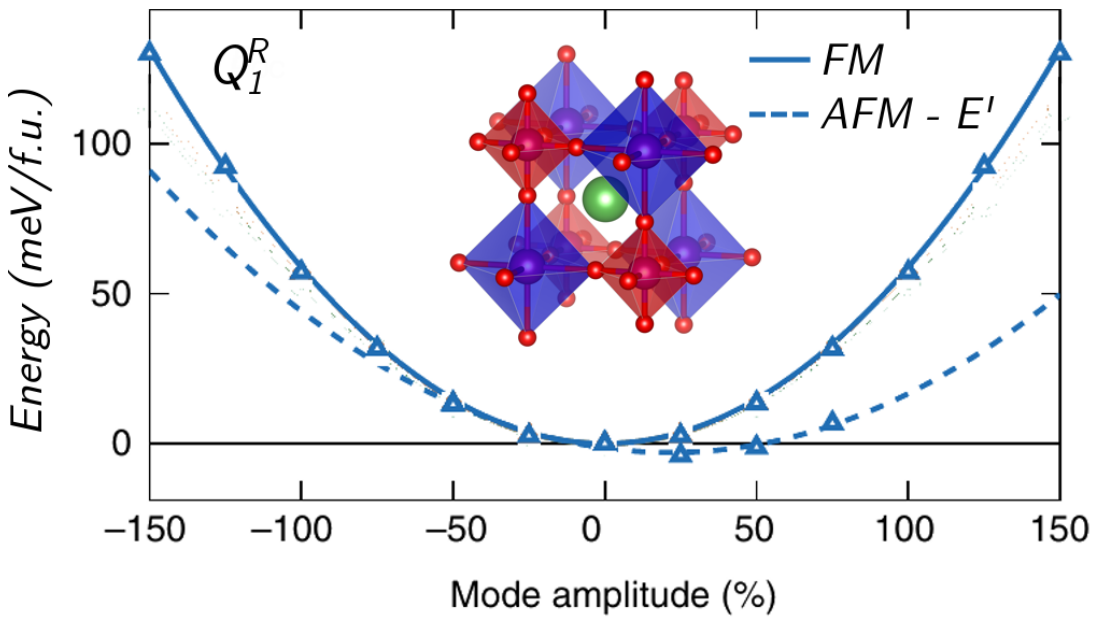
Q_1-Modes and Strains

Q_1 	$Q_1^{\mathbf{\Gamma}}$	$Q_1^{\mathbf{R}}$	$Q_{1\alpha}^{\mathbf{X}}$ 	$Q_{1\alpha}^{\mathbf{M}}$ 
Origin in A	$\Gamma_1^+\ (a)$	$R_2^-\ (a)$	$X_3^-\ (a,0,0)$	$M_4^+\ (a,0,0)$
Ref. $Pm\bar{3}m$ B	$\Gamma_1^+\ (a)$	$R_1^+\ (a)$	$X_1^+\ (a,0,0)$	$M_1^+\ (a,0,0)$
Displacement Pattern				
Strain Vector	$(a,a,a,0,0,0)$	-	-	-
Crystal Space Group (Schönflies)	$Pm\bar{3}m$ (O_h^1)	$Fm\bar{3}m$ (O_h^5)	$P4/mmm$ (D_{4h}^1)	$P4/mmm$ (D_{4h}^1)
Local Octahedral Symmetry	O_h	O_h	D_{4h}	D_{4h}

Schmitt, M. M., et al, arXiv:1909.06287 (2019)

Q_1-Modes and Strains

Q_1 			$Q_{1\alpha}^{\mathrm{M}}$ 
Origin in A Ref. $Pm\bar{3}m$ B			M_4^+ $(a,0,0)$ M_1^+ $(a,0,0)$
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

Schmitt, M. M., et al, arXiv:1909.06287 (2019)

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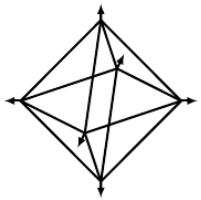
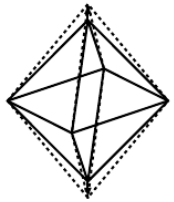
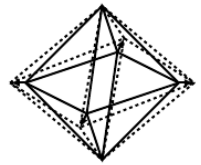
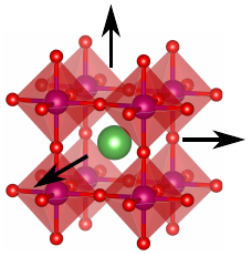
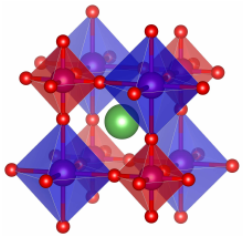
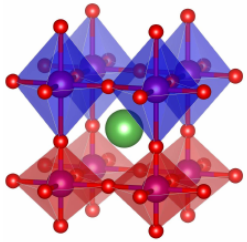
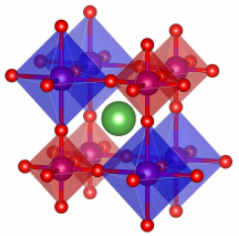
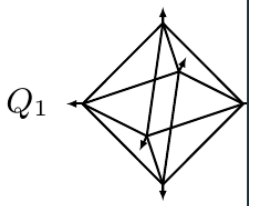
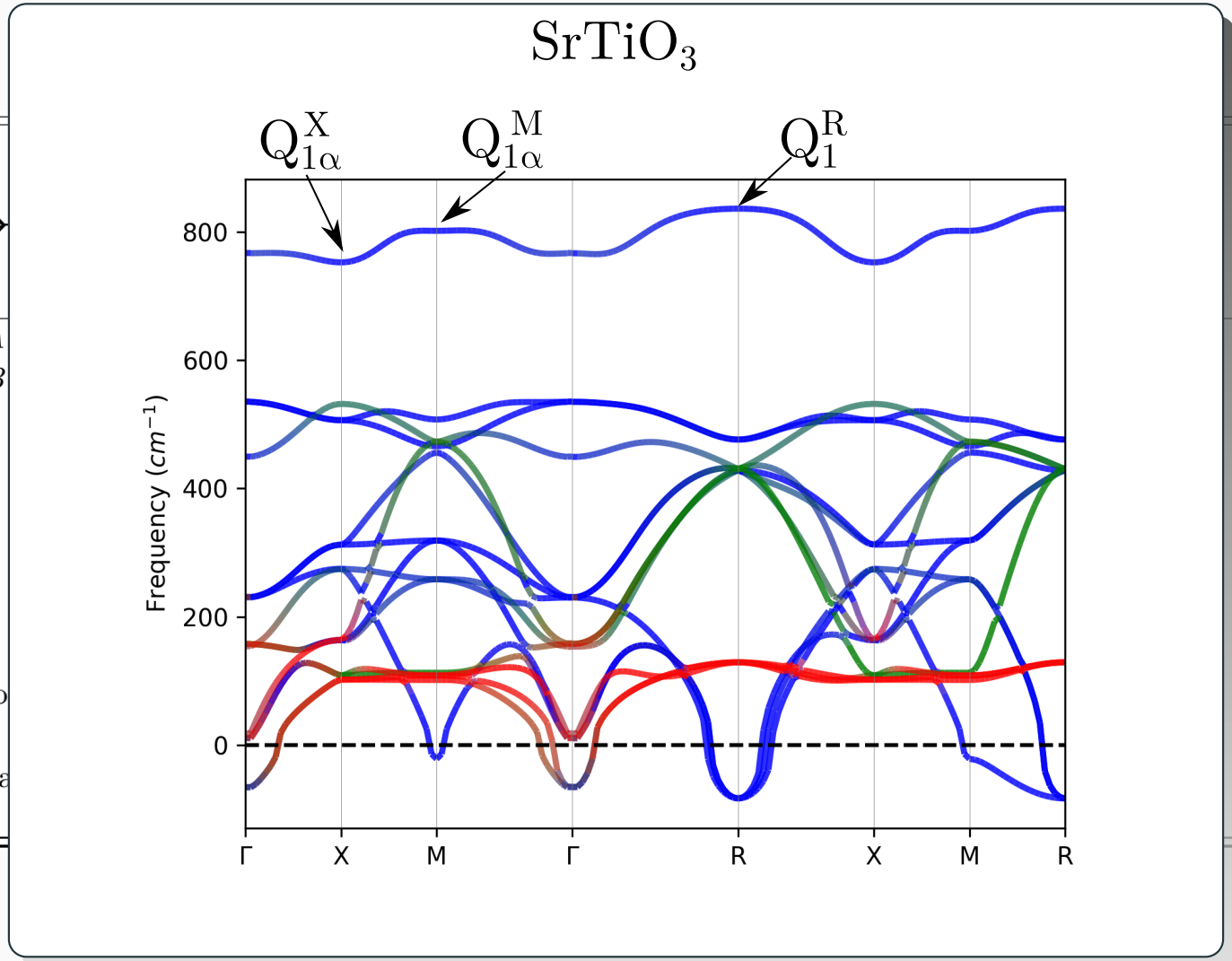
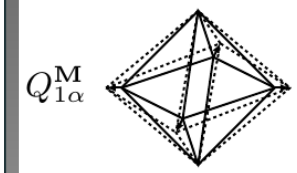
Q_1 	$Q_1^{\mathbf{\Gamma}}$	$Q_1^{\mathbf{R}}$	$Q_{1\alpha}^{\mathbf{X}}$ 	$Q_{1\alpha}^{\mathbf{M}}$ 
Origin in A	$\Gamma_1^+\ (a)$	$R_2^-\ (a)$	$X_3^-\ (a,0,0)$	$M_4^+\ (a,0,0)$
Ref. $Pm\bar{3}m$ B	$\Gamma_1^+\ (a)$	$R_1^+\ (a)$	$X_1^+\ (a,0,0)$	$M_1^+\ (a,0,0)$
Displacement Pattern				
Strain Vector	$(a,a,a,0,0,0)$	-	-	-
Crystal Space Group (Schönflies)	$Pm\bar{3}m$ (O_h^1)	$Fm\bar{3}m$ (O_h^5)	$P4/mmm$ (D_{4h}^1)	$P4/mmm$ (D_{4h}^1)
Local Octahedral Symmetry	O_h	O_h	D_{4h}	D_{4h}

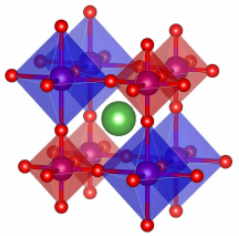
Schmitt, M. M., et al, arXiv:1909.06287 (2019)

Q_1-Modes and Strains



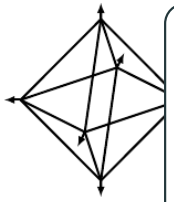
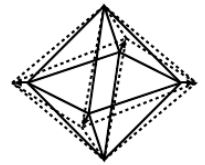
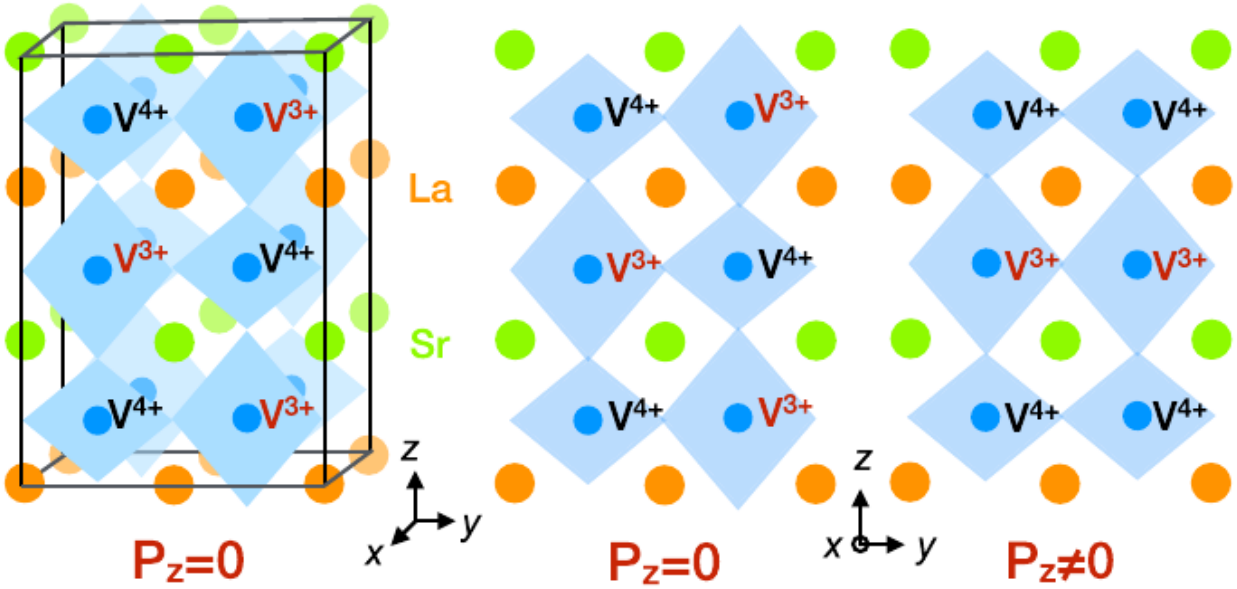
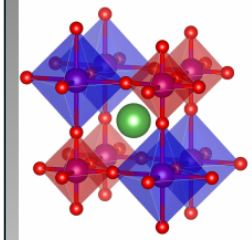




Origin in Ref.	A $Pm\bar{3}m$ B	M_4^+ $(a,0,0)$ M_1^+ $(a,0,0)$
Displacement Pattern		
Strain Vector		-
Crystal Space Gro (Schönflies)		$P4/mmm$ (D^1_{4h})
Local Octahedra Symmetry		D_{4h}

Schmitt, M. M., et al, arXiv:1909.06287 (2019)

Q_1-Modes and Strains

Q_1			$Q^{\mathrm{M}}_{1\alpha}$ 
Origin in Ref. $Pm\bar{3}m$			$M_4^+\ (a,0,0)$ $M_1^+\ (a,0,0)$
Displacement Pattern			
Strain Vector			-
Crystal Space Gr (Schönflies)			$P4/mmm$ (D^1_{4h})
Local Octahedr Symmetry			D_{4h}

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

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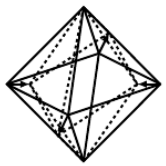
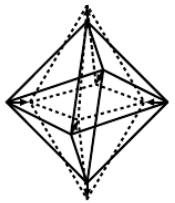
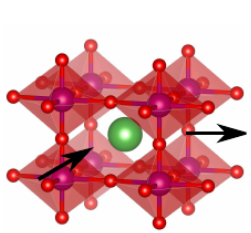
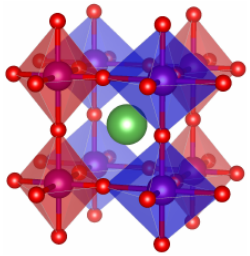
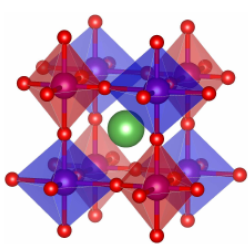
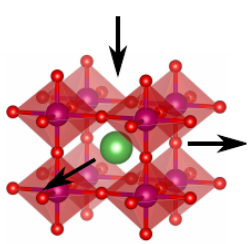
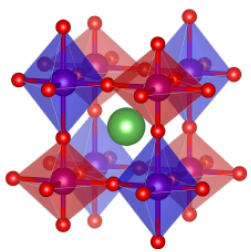
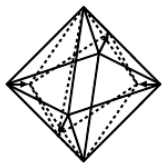
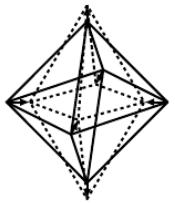
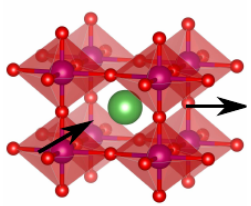
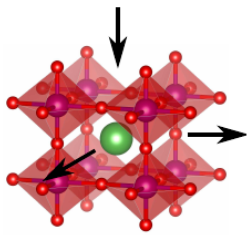
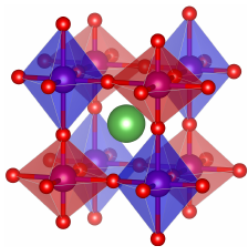
Q_2/Q_3-Modes and Strains

Q_2 	$Q_{2\alpha}^{\mathbf{\Gamma}}$	$Q_{2\alpha}^{\mathbf{M}}$	$Q_{2\alpha}^{\mathbf{R}}$	Q_3 	$Q_{3\alpha}^{\mathbf{\Gamma}}$	$Q_{3\alpha}^{\mathbf{R}}$
Origin in A	$\Gamma_3^+\ (0,a)$	$M_3^+\ (a,0,0)$	$R_3^-\ (0,a)$		$\Gamma_3^+\ (a,0)$	$R_3^-\ (a,0)$
Ref. $Pm\bar{3}m$ B	$\Gamma_3^+\ (0,a)$	$M_2^+\ (a,0,0)$	$R_3^+\ (0,a)$		$\Gamma_3^+\ (a,0)$	$R_3^+\ (a,0)$
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}

Schmitt, M. M., et al, arXiv:1909.06287 (2019)

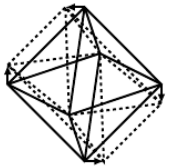
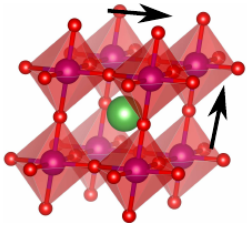
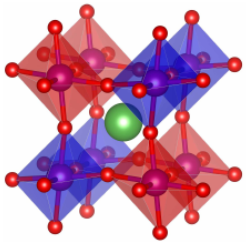
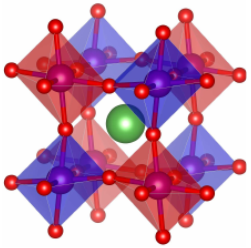
Q_2/Q_3-Modes and Strains

Q_2 	$Q^{\Gamma}_{2\alpha}$	$Q^{\mathbf{M}}_{2\alpha}$	$Q^{\mathbf{R}}_{2\alpha}$	Q_3 	$Q^{\Gamma}_{3\alpha}$	$Q^{\mathbf{R}}_{3\alpha}$
Origin in A	$\Gamma_3^+\ (0,a)$	$M_2^+\ (a,0,0)$	$R_2^-\ (0,a)$		$\Gamma_3^+\ (a,0)$	$R_3^-\ (a,0)$
Ref. $Pm\bar{3}m$ B	$\Gamma_3^+\ (0,a)$				$\Gamma_3^+\ (a,0)$	$R_3^+\ (a,0)$
Displacement Pattern						
Strain Vector	$(0,-a,a,0,0,0)$	-	-		$(-2a,a,a,0,0,0)$	-
Crystal Space Group (Schönflies)	$Pmmm$ (D^1_{2h})	$P4/mbm$ (D^5_{4h})	$I4/mcm$ (D^{18}_{4h})		$P4/mmm$ (D^1_{4h})	$I4/mmm$ (D^{17}_{4h})
Local Octahedral Symmetry	D_{2h}	D_{2h}	D_{2h}		D_{4h}	D_{4h}

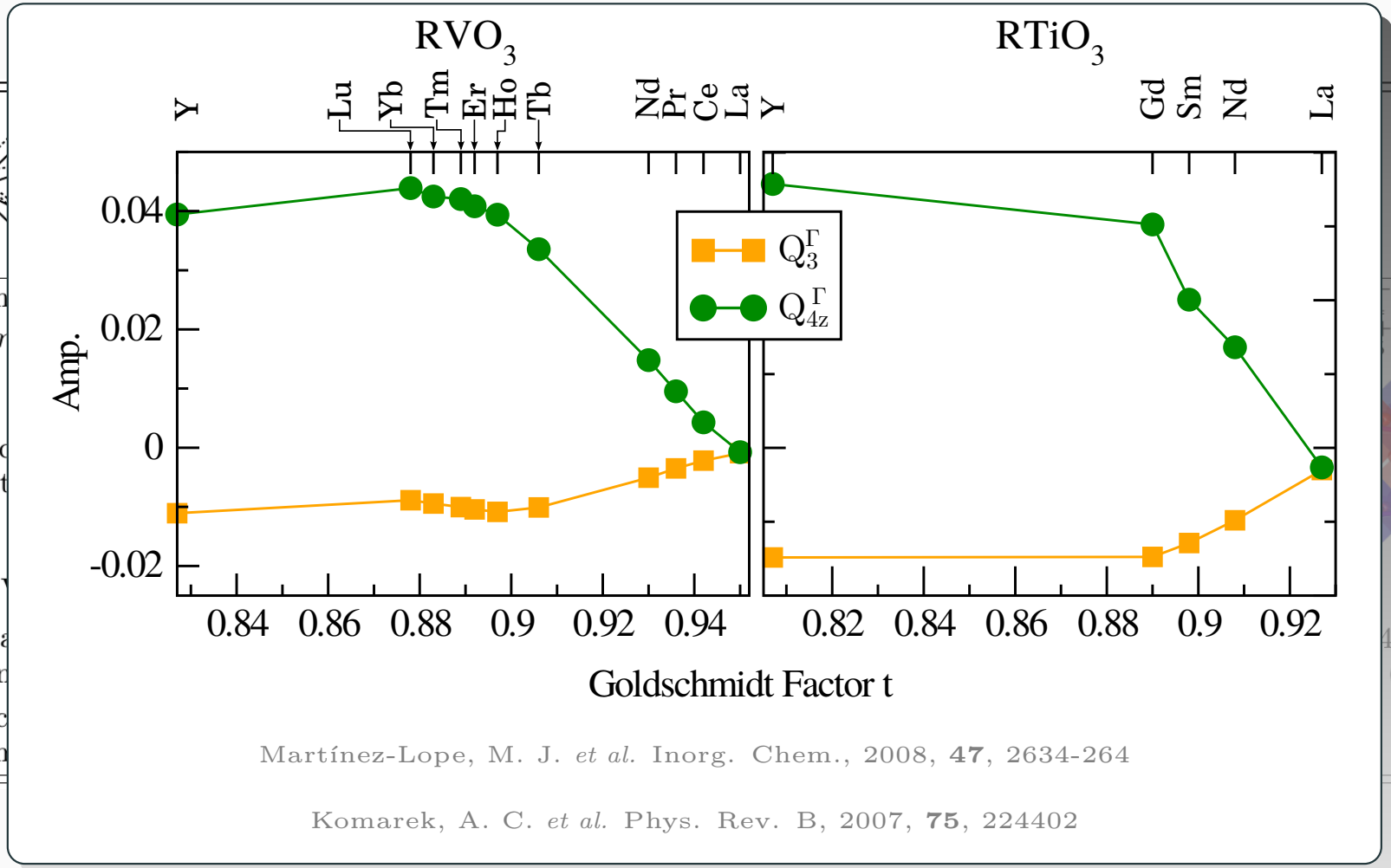
$RMnO_3$	$Q^{\mathbf{M}}_{2z}$ & Q^{Γ}_{3z}
$KCuF_3$	$Q^{\mathbf{R}}_{2z}$ & Q^{Γ}_{3z}
$KCrF_3$	$Q^{\mathbf{R}}_{2z}$ & Q^{Γ}_{3z}

Schmitt, M. M., et al, arXiv:1909.06287 (2019)

Q_4, Q_5, Q_6-Modes and Strains

$Q_{4,5,6}$ 	$Q^{\mathbf{\Gamma}}_{4\alpha}$	$Q^{\mathbf{M}}_{4\alpha}$	$Q^{\mathbf{R}}_{4\alpha}$
Origin in A	$\Gamma_5^+\ (a,0,0)$	$M_1^+\ (a,0,0)$	$R_4^-\ (a,0,0)$
Ref. $Pm\bar{3}m$ B	$\Gamma_5^+\ (a,0,0)$	$M_4^+\ (a,0,0)$	$R_5^+\ (a,0,0)$
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

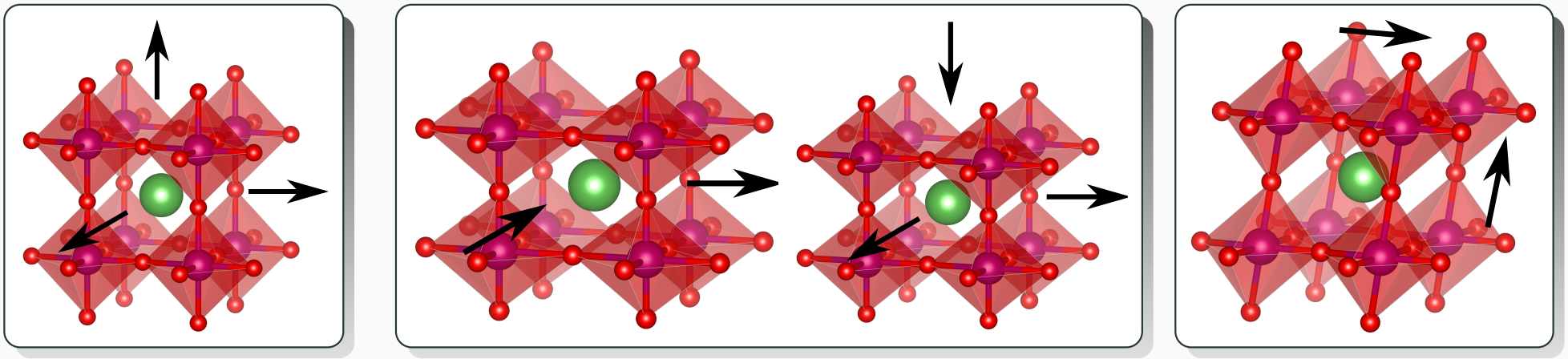


Martínez-Lope, M. J. *et al.* Inorg. Chem., 2008, **47**, 2634-264

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

CJTN - Strain Basis

$\mathbf{a_{1g}}$ Q_1^Γ | $\mathbf{e_g}$ $Q_{2\alpha}^\Gamma$ & $Q_{3\alpha}^\Gamma$ | $\mathbf{t_{2g}}$ $Q_{4x,y,z}^\Gamma$



$$\hat{=} \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ & \epsilon_{yy} & \epsilon_{yz} \\ sym & & \epsilon_{zz} \end{pmatrix} \hat{=} (\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4, \epsilon_5, \epsilon_6)$$

Schmitt, M. M., et al, arXiv:1909.06287 (2019)

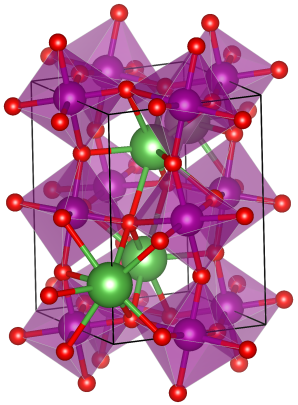
Application I: Bulk Ground State of $LaMnO_3$

JTD In $LaMnO_3$

GS

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

+ JTD

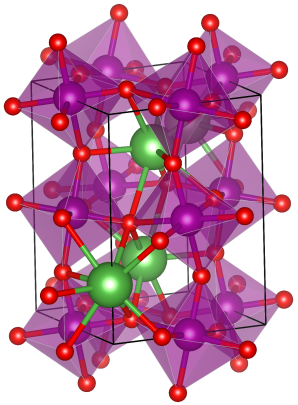


JTD In $LaMnO_3$

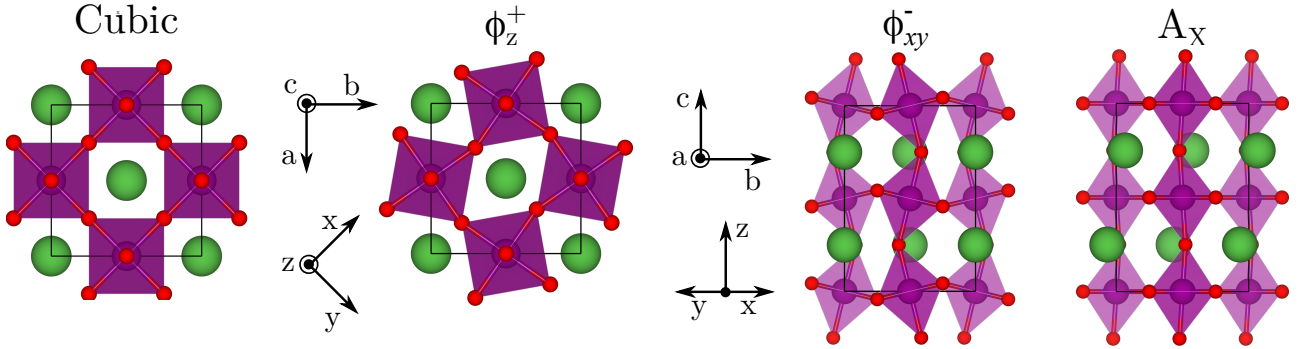
GS

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

+ JTD



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

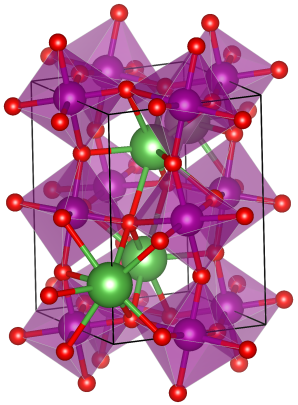


JTD In $LaMnO_3$

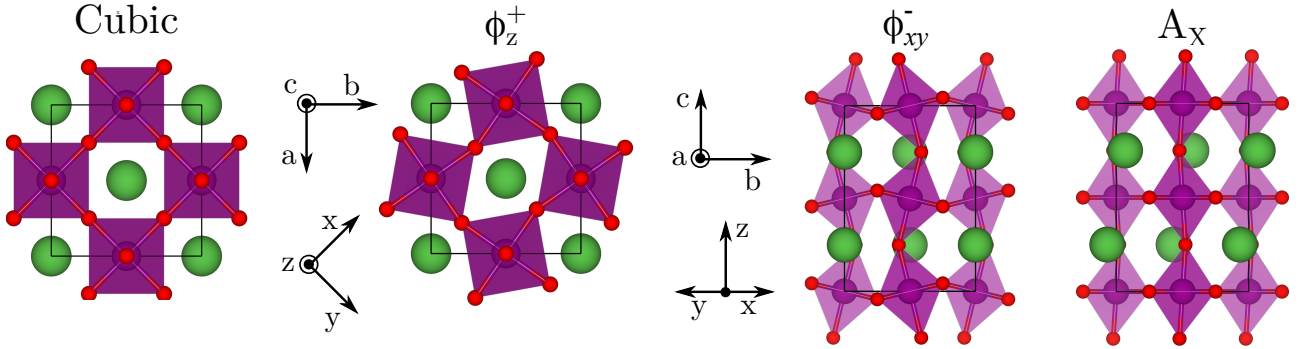
GS

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

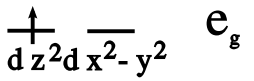
+ JTD

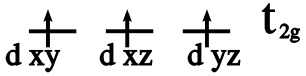


Metallic O-Phase $750K < T < 1200K$



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



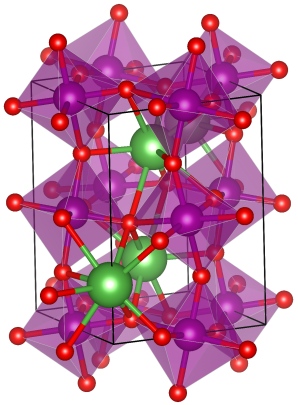


JTD In $LaMnO_3$

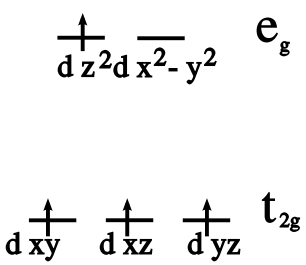
GS

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

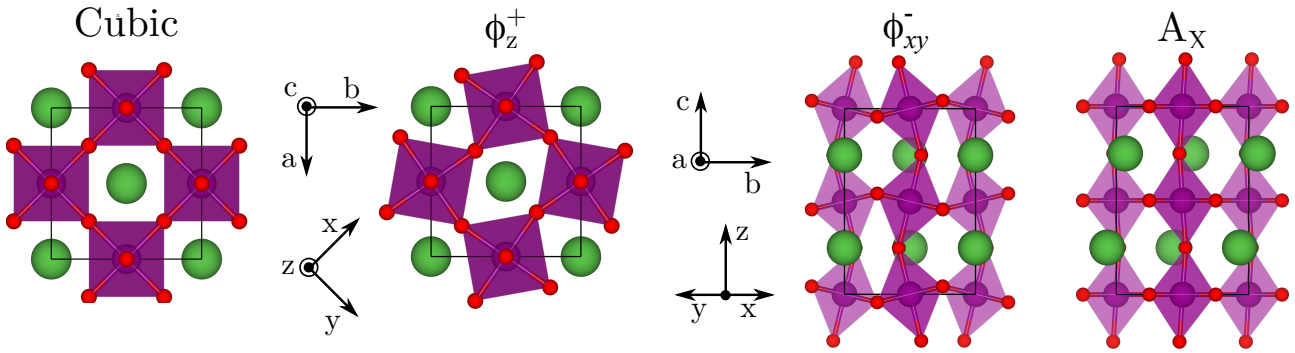
+ JTD



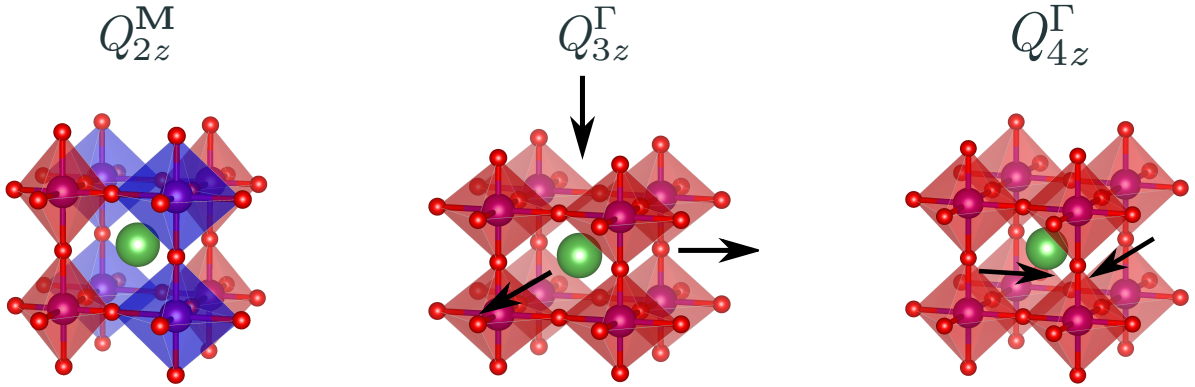
$\mathbf{Mn^{3+} = d^4}$



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



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

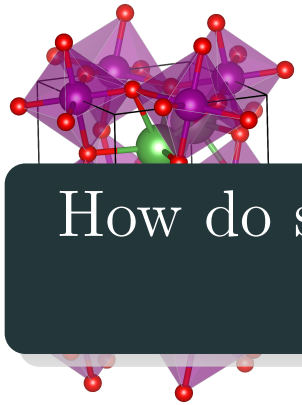


JTD In $LaMnO_3$

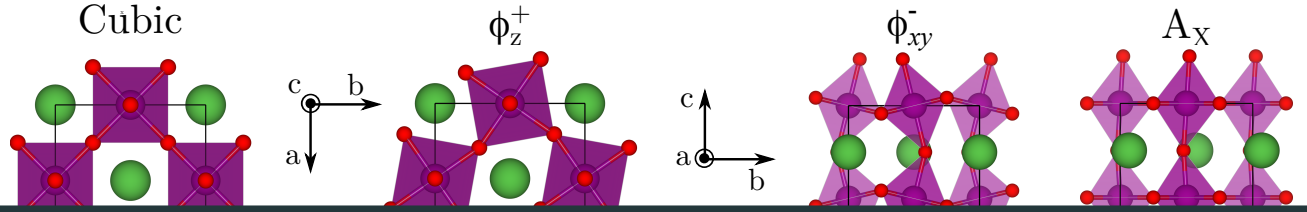
GS

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

+ JTD



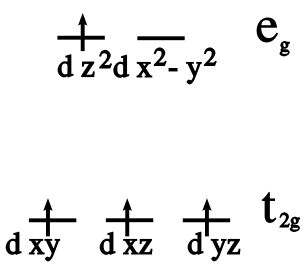
Metallic O-Phase $750K < T < 1200K$



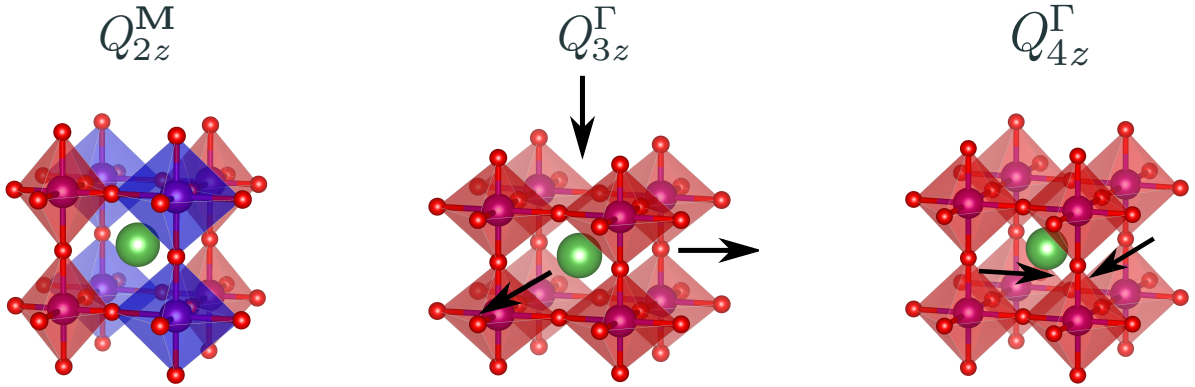
How do structural and electronic degrees of freedom interact ?

Let's ask DFT!

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



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

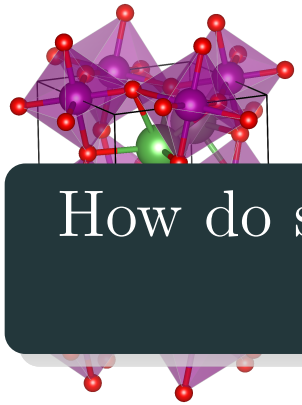


JTD In $LaMnO_3$

GS

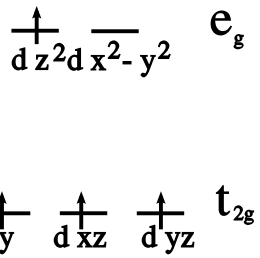
$Pnma\ a^-a^-c^+$

+ JTD



How do stru

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



b-initio VASP ienna ackage imulation

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 ✓

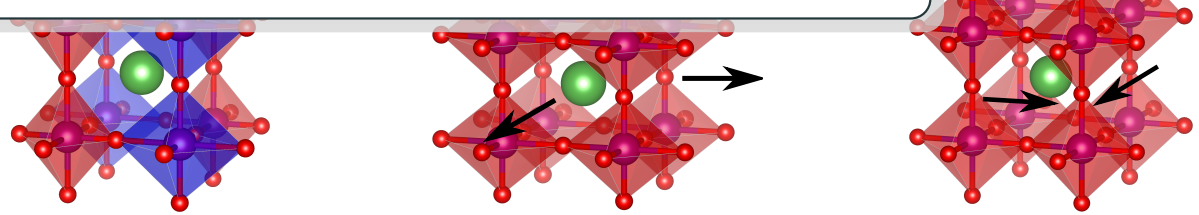
200K

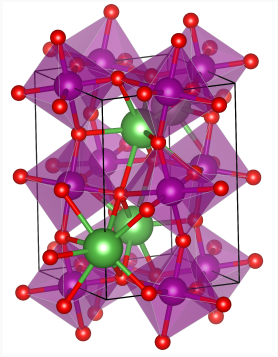
A_X

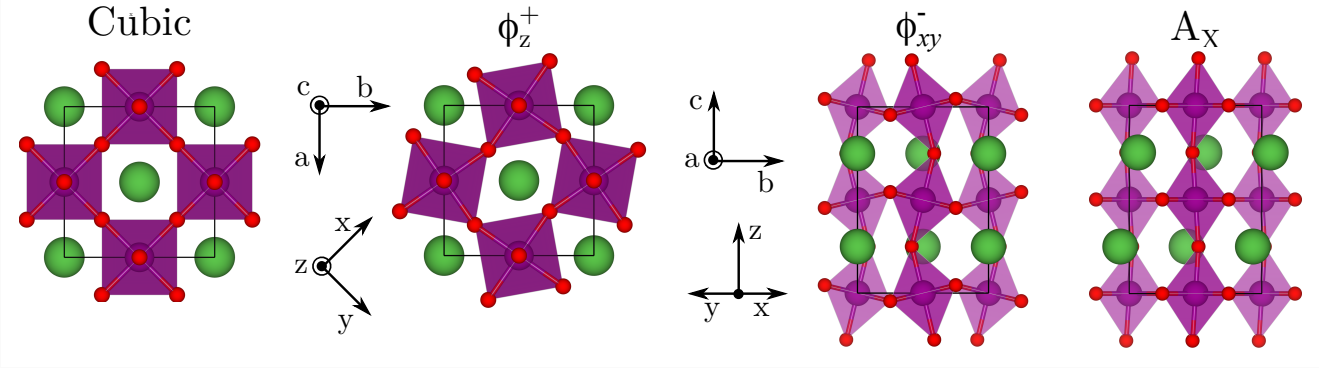
n interact ?

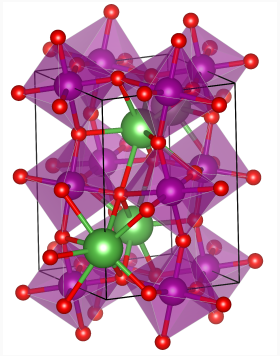
A T < 140K

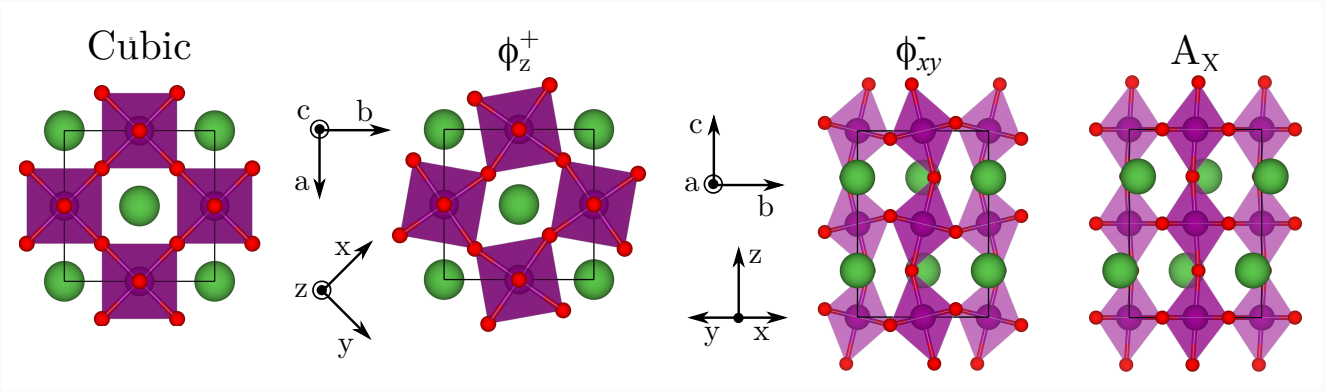
Q^{Γ}_{4z}

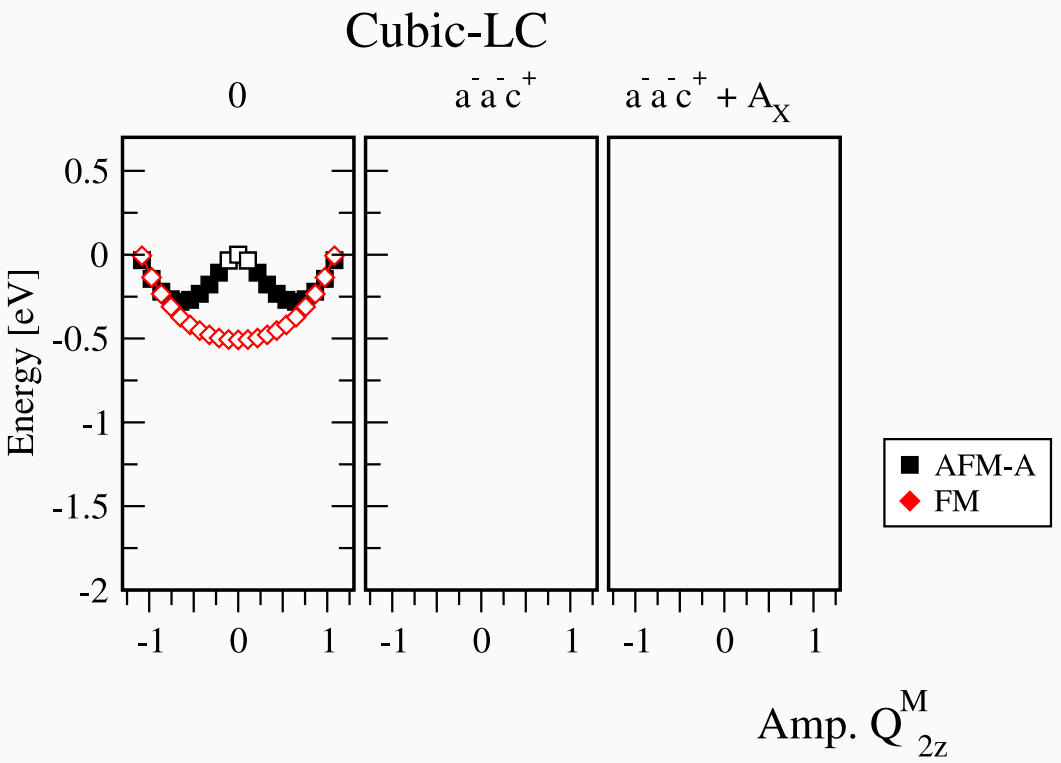




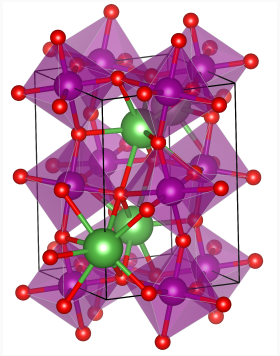

Cubic
ϕ_z^+
ϕ_{xy}^-
A_X
c
b
a
x
z
y
c
a
b
z
y
x

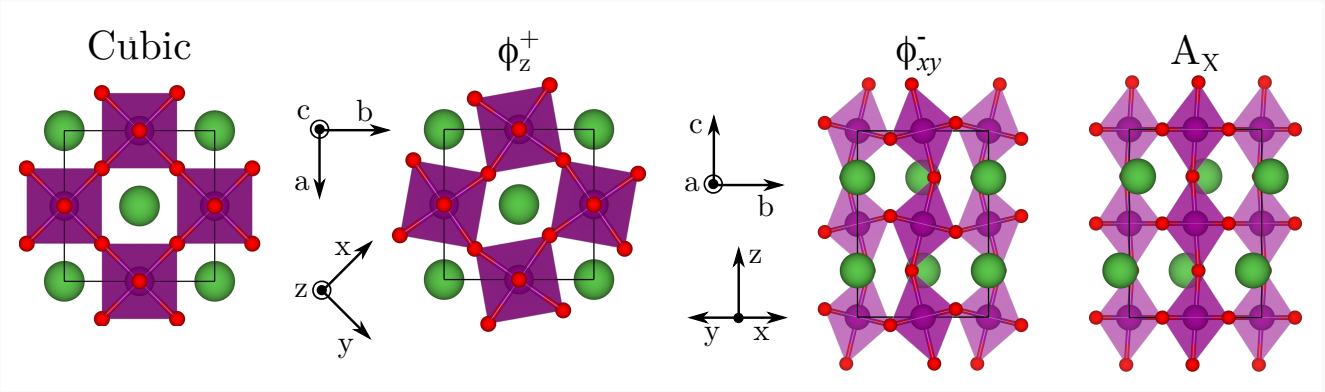


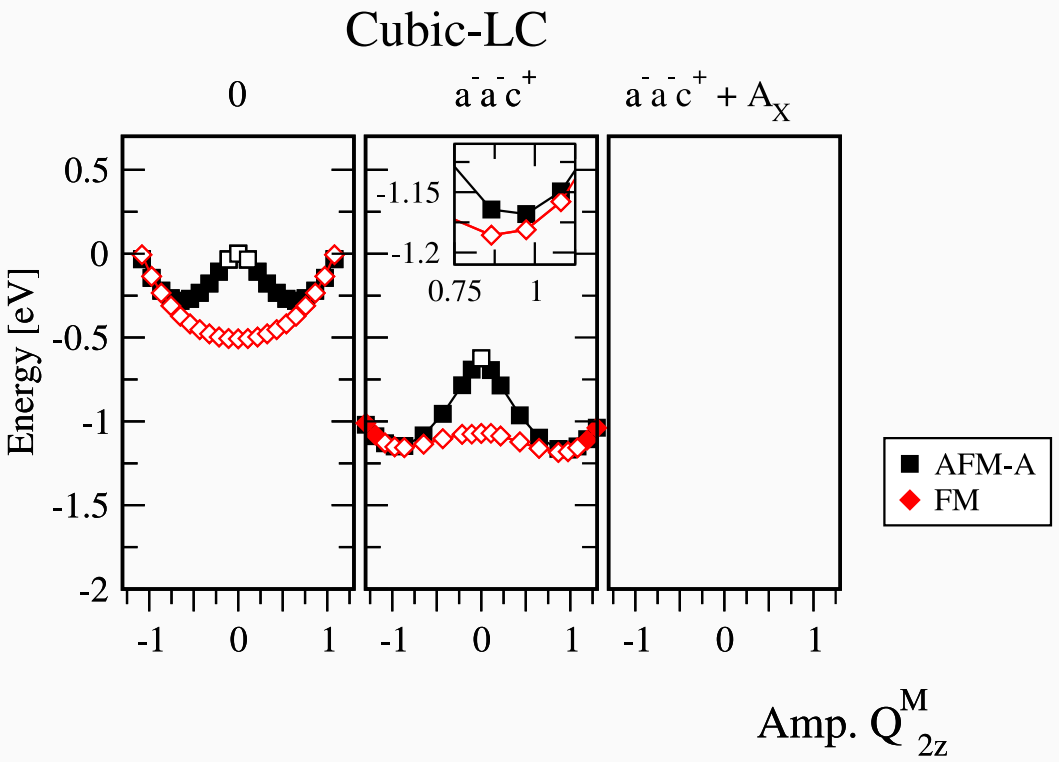




$$F \propto \alpha_{el} Q_{2z}^{M} + \beta_1 Q_{2z}^{M^2}$$

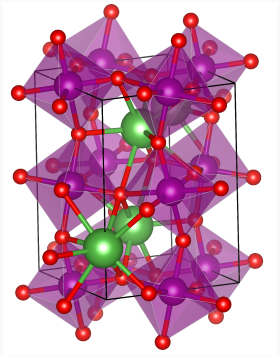


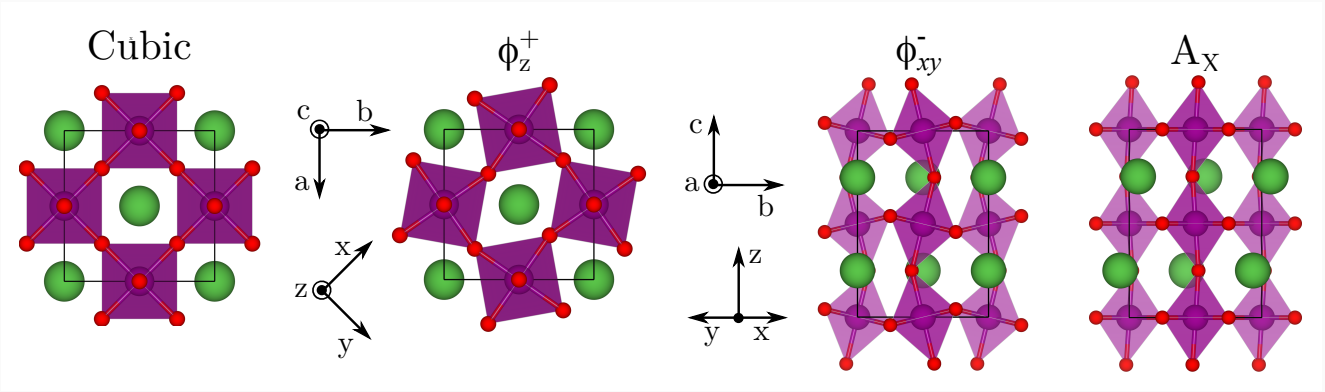


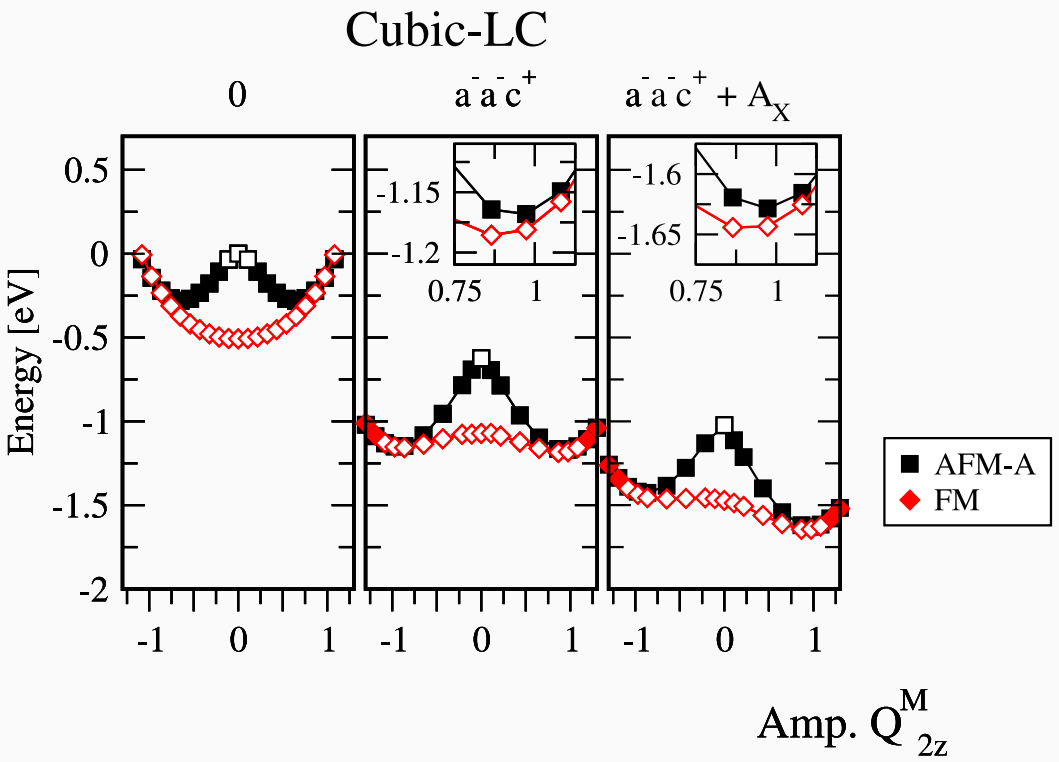


$$F \propto \alpha_{el} Q_{2z}^M + \beta_1 Q_{2z}^{M^2} + \beta_2 \phi^2 Q_{2z}^{M^2}$$

$$\beta_2 < 0$$

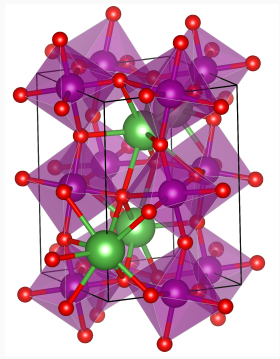


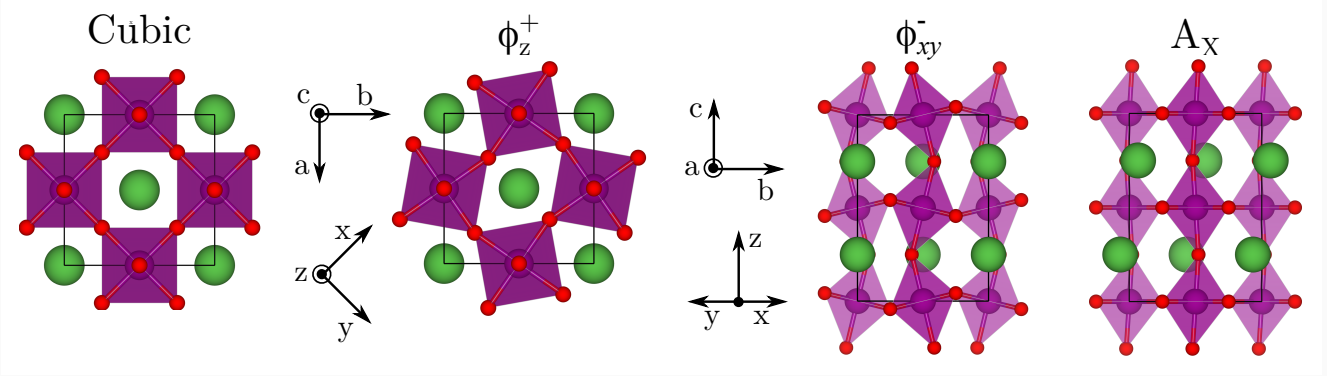


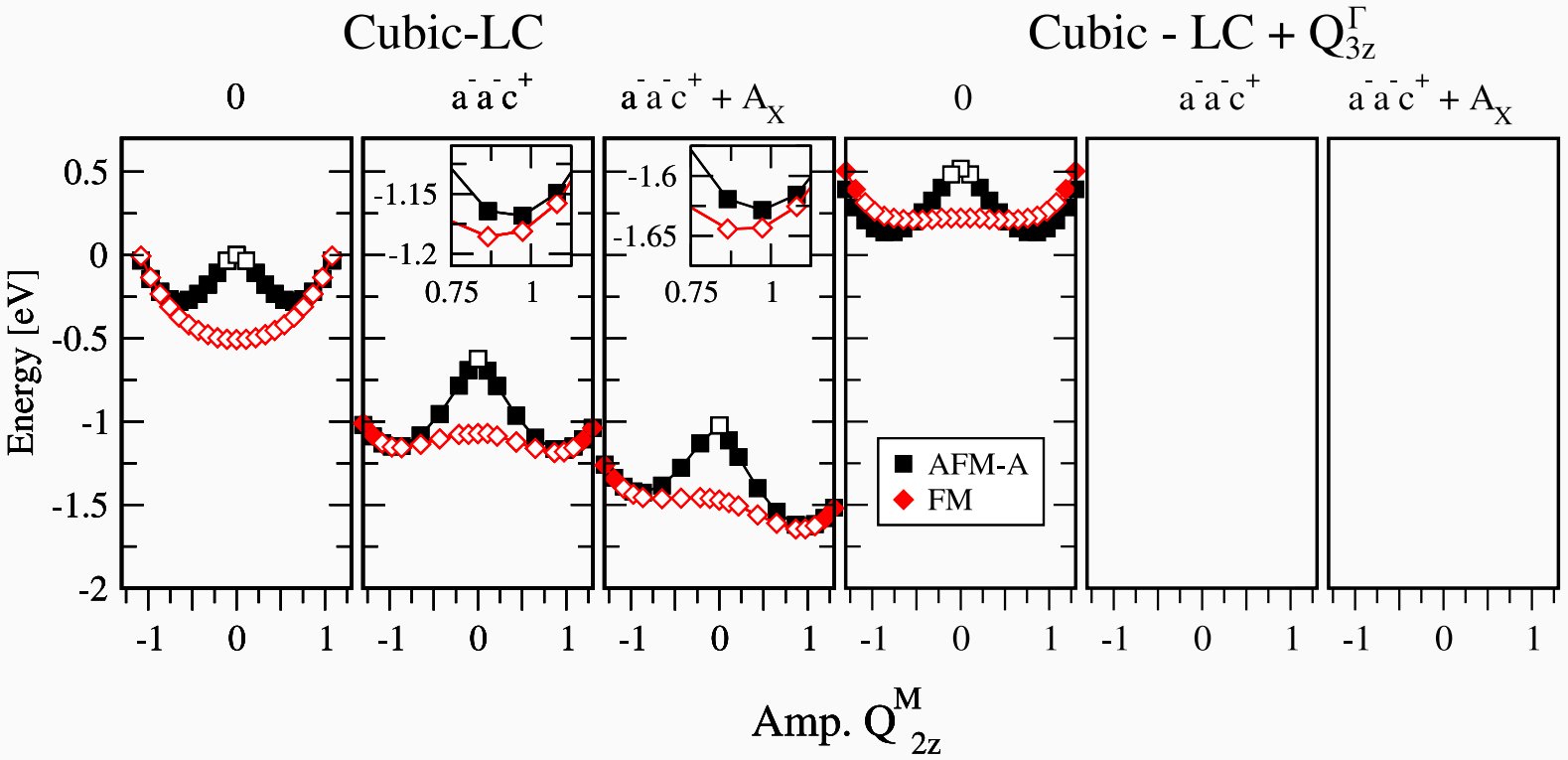


$$F \propto \alpha_{el} Q_{2z}^M + \beta_1 Q_{2z}^{M^2} + \beta_2 \phi^2 Q_{2z}^{M^2} + \gamma_1 A_X \phi^- Q_{2z}^M$$

$$\beta_2 < 0$$

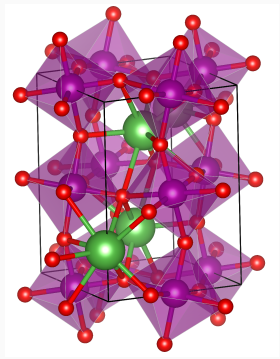


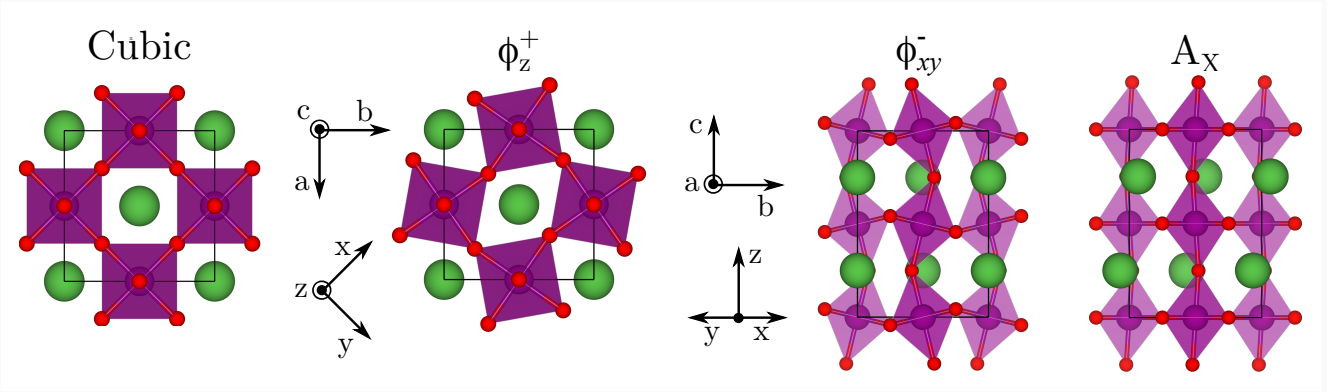


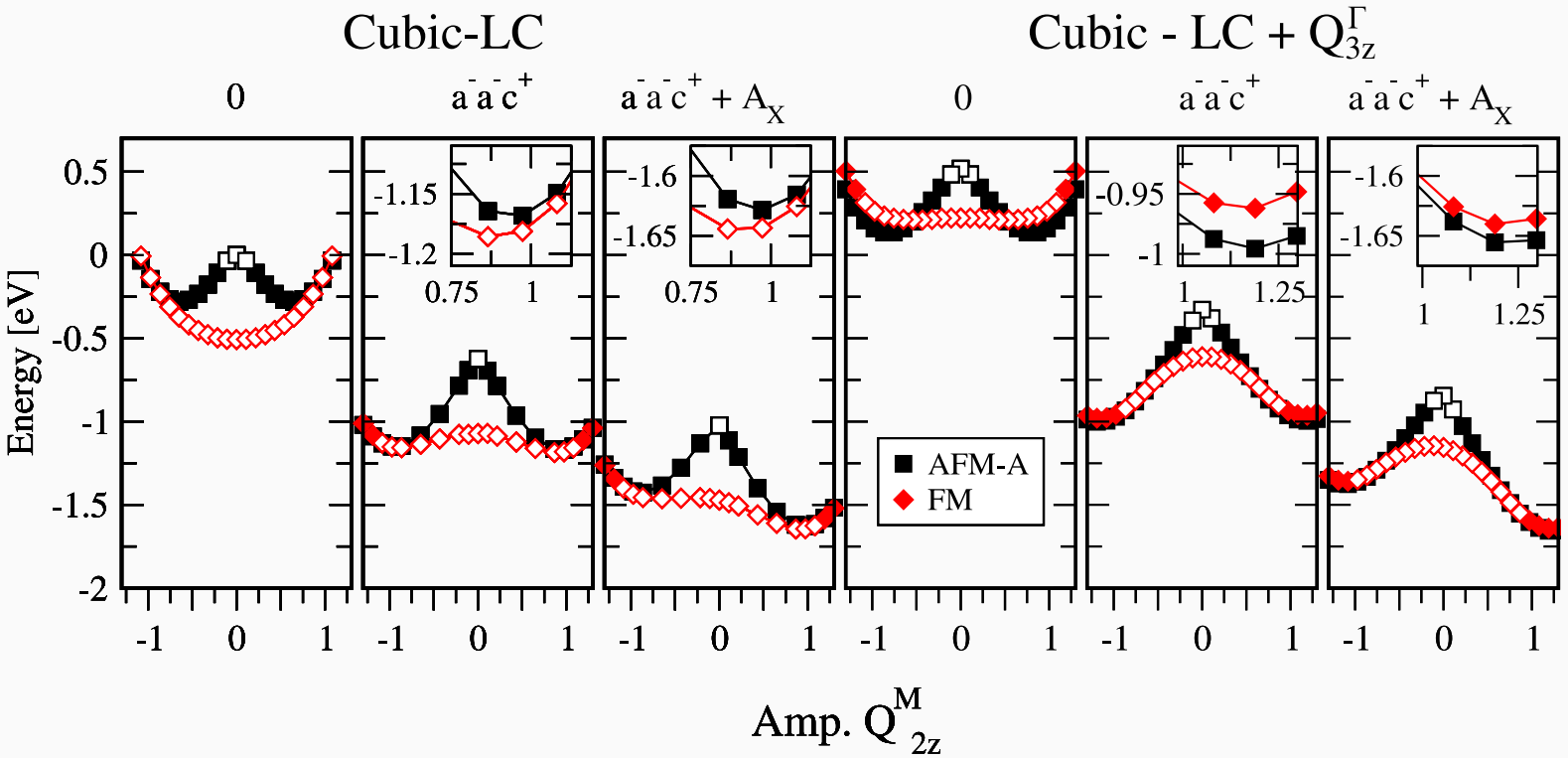


$$F \propto \alpha_{el} Q_{2z}^{M} + \beta_1 Q_{2z}^{M^2} + \beta_2 \phi^2 Q_{2z}^{M^2} + \gamma_1 A_X \phi^- Q_{2z}^{M} + \beta_3 Q_{3z}^{\Gamma} Q_{2z}^{M^2} + \beta_4 Q_{3z}^{\Gamma^2} Q_{2z}^{M^2}$$

$$|\beta_3| > |\beta_4|$$

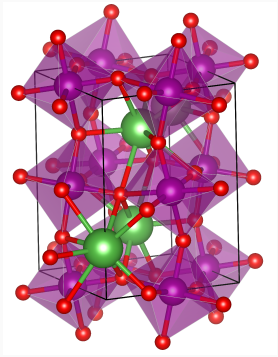


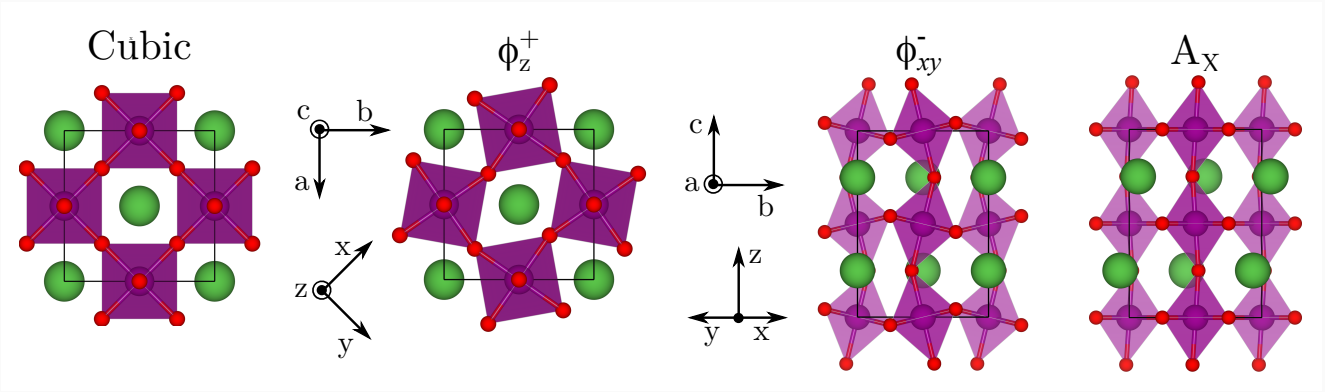


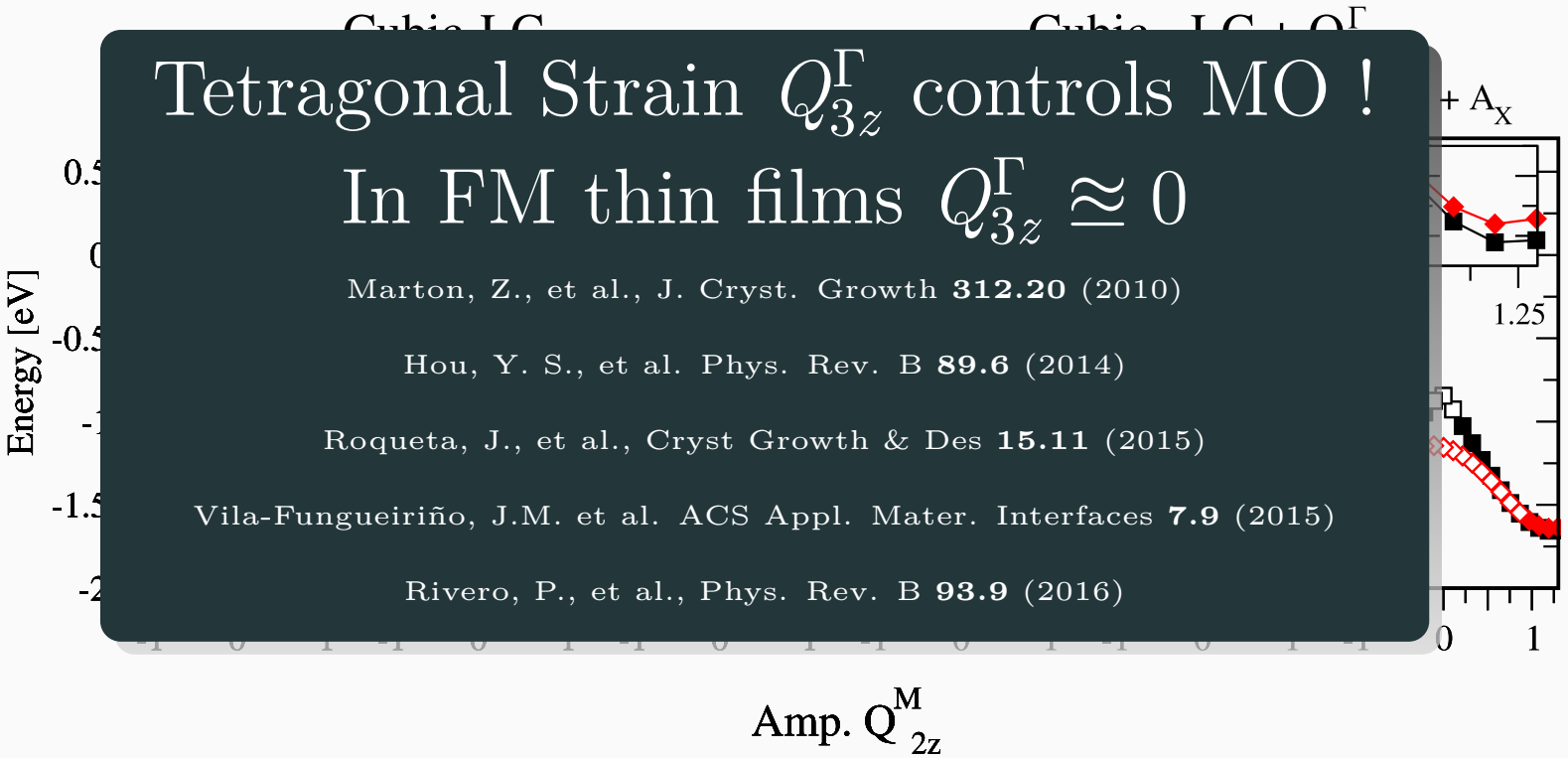


$$F \propto \alpha_{el} Q_{2z}^{M} + \beta_1 Q_{2z}^{M^2} + \beta_2 \phi^2 Q_{2z}^{M^2} + \gamma_1 A_X \phi^- Q_{2z}^{M} + \beta_3 Q_{3z}^{\Gamma} Q_{2z}^{M^2} + \beta_4 Q_{3z}^{\Gamma^2} Q_{2z}^{M^2}$$

$$|\beta_3| > |\beta_4|$$







Tetragonal Strain Q^Γ_{3z} controls MO !

In FM thin films $Q^\Gamma_{3z} \approx 0$

Marton, Z., et al., J. Cryst. Growth **312.20** (2010)

Hou, Y. S., et al. Phys. Rev. B **89.6** (2014)

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

Vila-Fungueiriño, J.M. et al. ACS Appl. Mater. Interfaces **7.9** (2015)

Rivero, P., et al., Phys. Rev. B **93.9** (2016)

$$F \propto \alpha_{el} Q_{2z}^M + \beta_1 Q_{2z}^{M^2} + \beta_2 \phi^2 Q_{2z}^{M^2} + \gamma_1 A_X \phi^- Q_{2z}^M + \beta_3 Q_{3z}^\Gamma Q_{2z}^{M^2} + \beta_4 Q_{3z}^{\Gamma^2} Q_{2z}^{M^2}$$

$$|\beta_3| > |\beta_4|$$

Application II: [001] Epitaxial Strain Phase Diagram of $CaFeO_3$

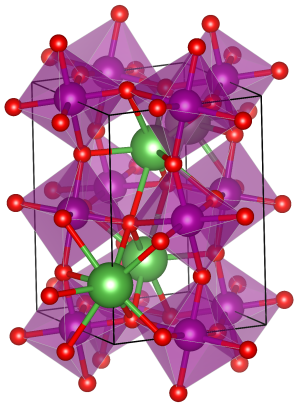
GS of $CaFeO_3$

GS

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

$+\ Q_1^{\mathbf{R}}$

$\rightarrow P2_1/n$



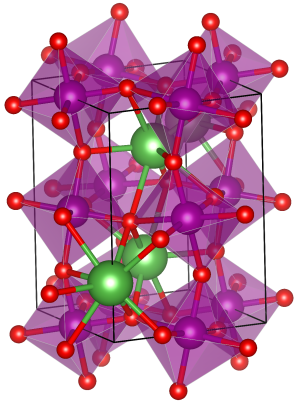
GS of $CaFeO_3$

GS

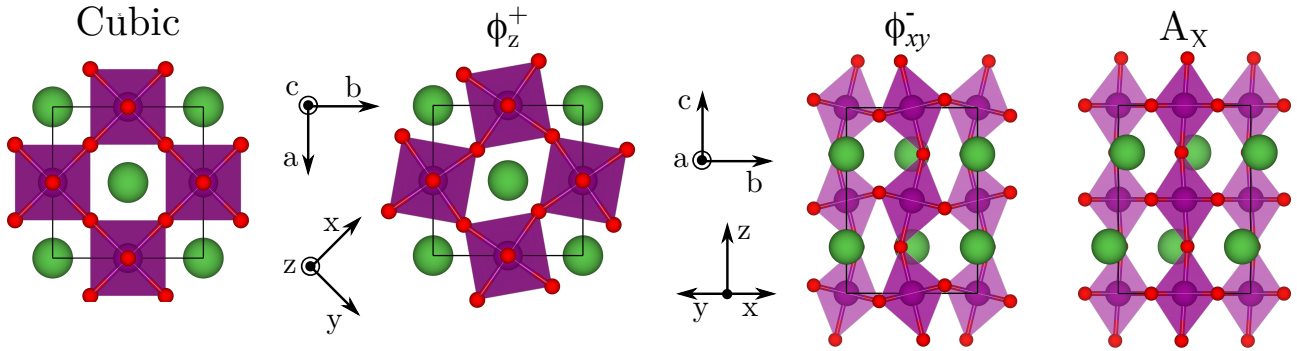
$Pnma\ a^-a^-c^+$

$+\ Q_1^{\mathbf{R}}$

$\rightarrow P2_1/n$



Metallic $Pnma\ T > 290K$



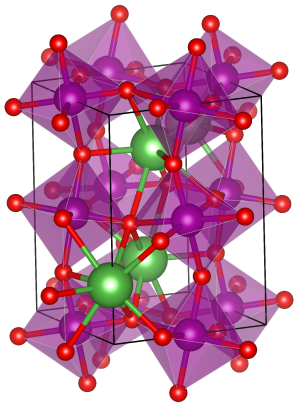
GS of $CaFeO_3$

GS

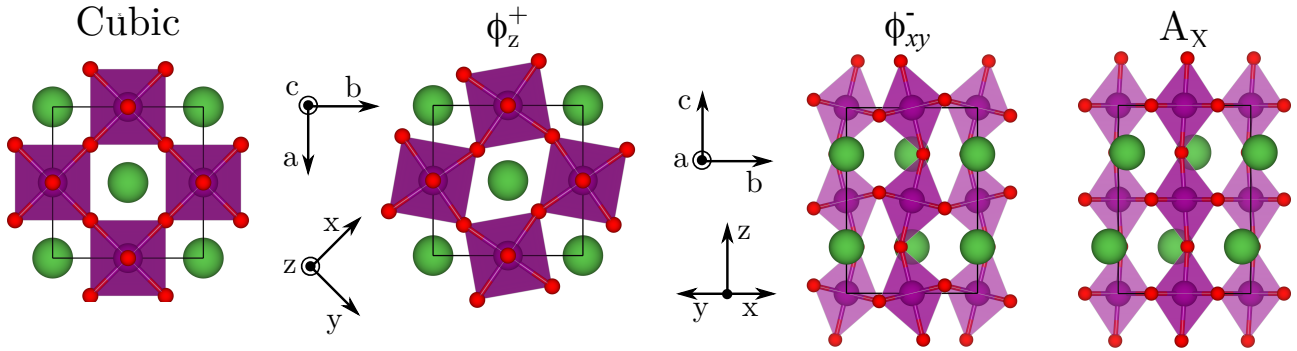
$Pnma\ a^-a^-c^+$

$+\ Q_1^{\mathbf{R}}$

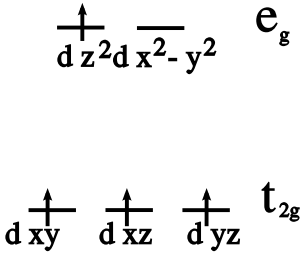
$\rightarrow P2_1/n$



Metallic $Pnma\ T > 290K$



$\mathbf{Fe^{4+} = d^4}$



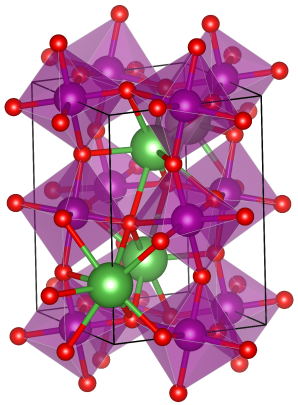
GS of $CaFeO_3$

GS

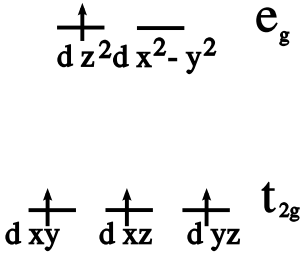
$Pnma\ a^-a^-c^+$

$+\ Q_1^{\mathbf{R}}$

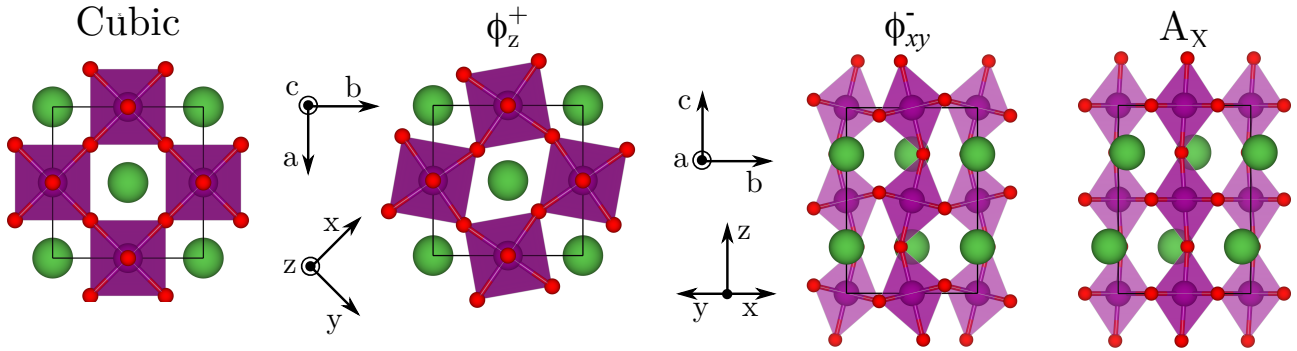
$\rightarrow P2_1/n$



$\mathbf{Fe^{4+} = d^4}$



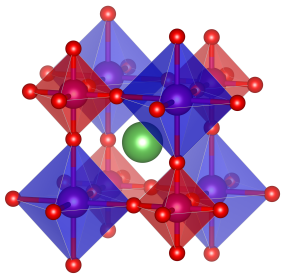
Metallic $Pnma\ T > 290K$



Ins. $P2_1/n\ T < T_{MIT} \approx 290K$

AFM T < 120K

$Q_1^{\mathbf{R}}$



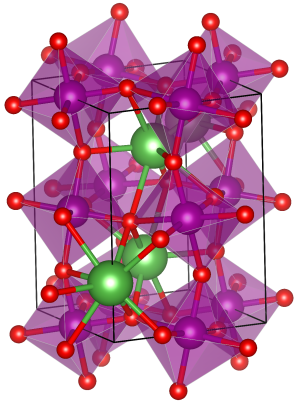
GS of $CaFeO_3$

GS

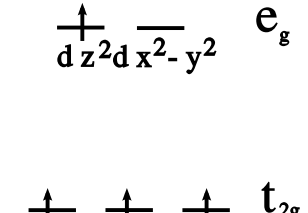
$Pnma\ a^-a^-c^+$

$+\ Q_1^{\mathbf{R}}$

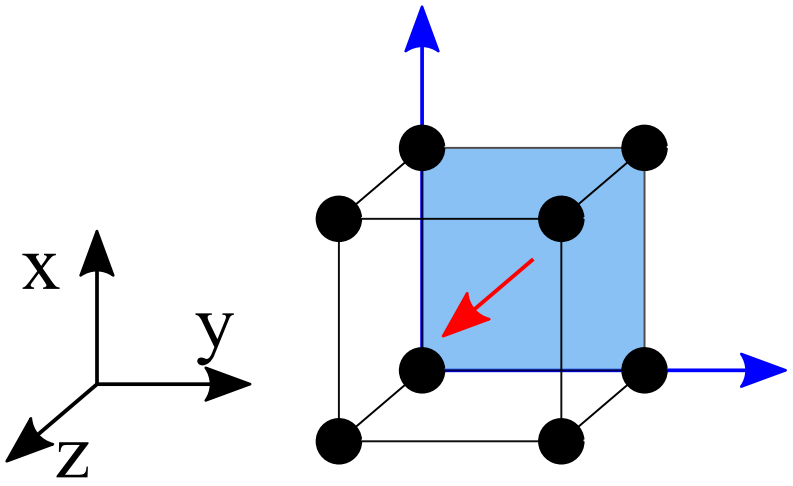
$\rightarrow P2_1/n$



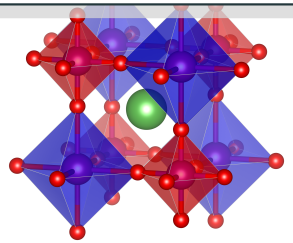
$\mathbf{Fe^{4+} = d^4}$

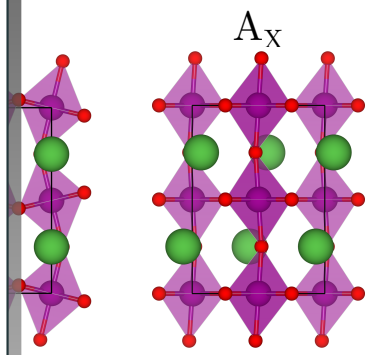


Effect of [001] epitaxial strain?



$\rightarrow Q_{3z}^{\Gamma} \neq 0$



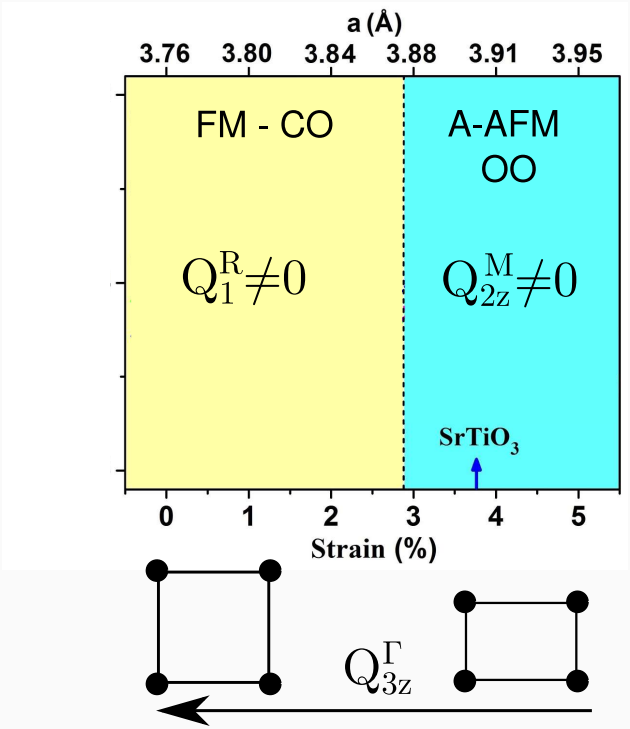


$0K$

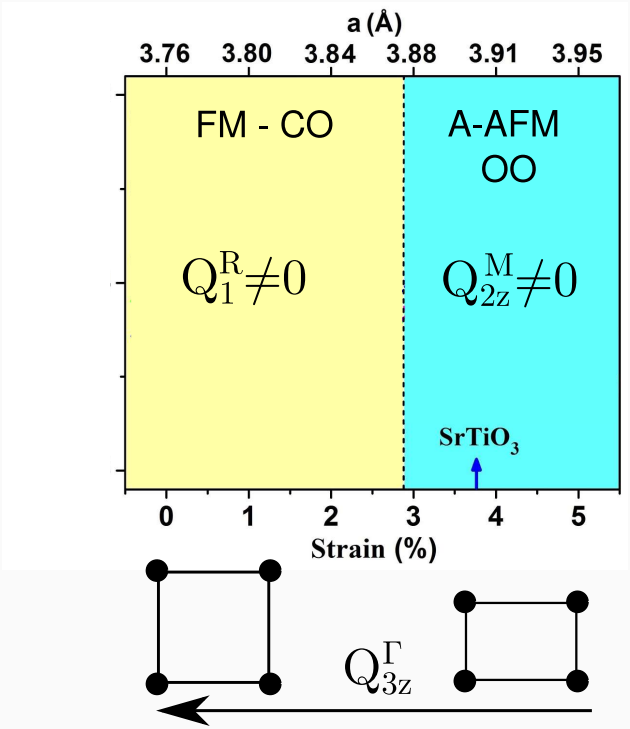
[001] Epitaxial Strain Tuning: *From Charge- to Orbital-Order*

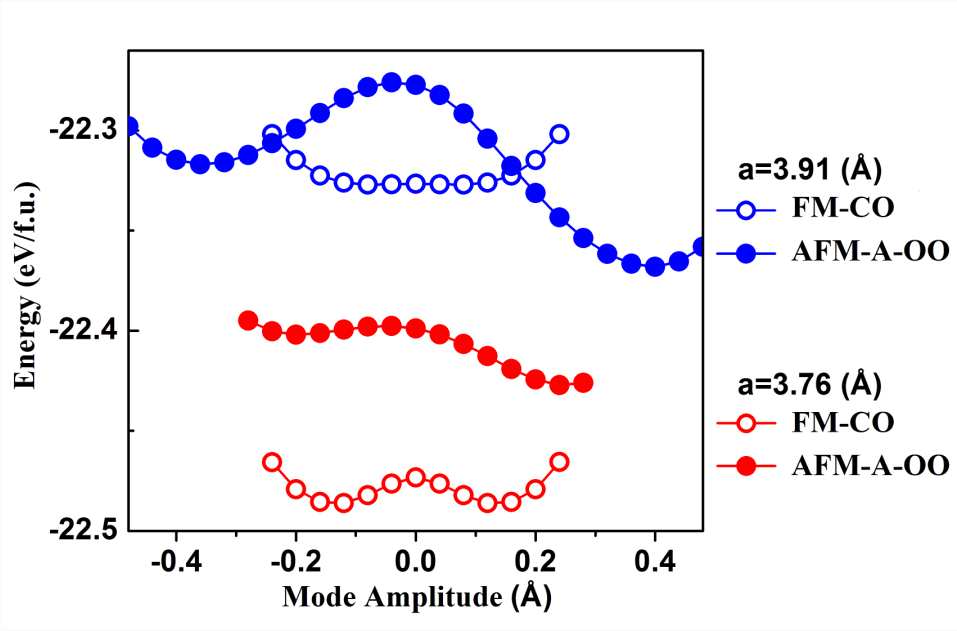
Zhang, Schmitt *et al.* Phys. Rev. B **98**, 081108(R), (2018)

[001] Epitaxial Strain Tuning: *From Charge- to Orbital-Order*



[001] Epitaxial Strain Tuning: *From Charge- to Orbital-Order*





$$F \propto \beta_3 Q_{3z}^{\Gamma} Q_{2z}^{M^2} + \beta_4 Q_{3z}^{\Gamma^2} Q_{2z}^{M^2}$$

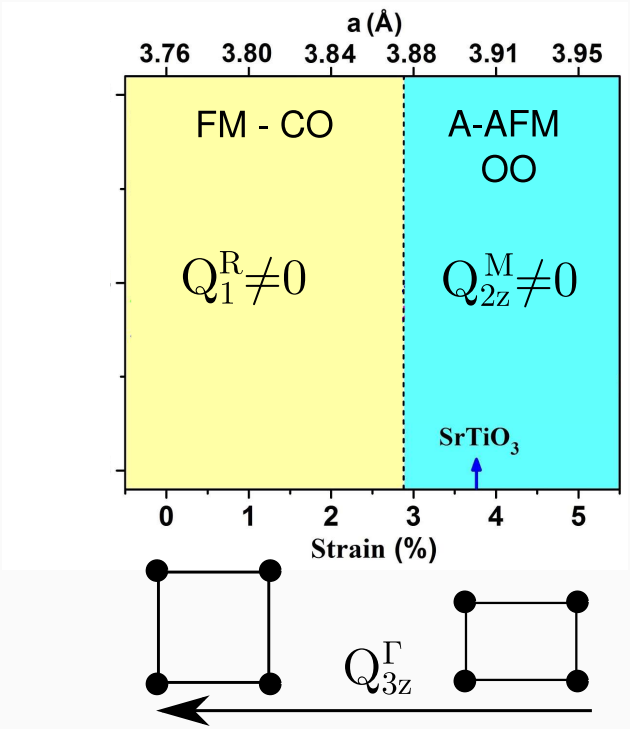
$$|\beta_3| >> |\beta_4|$$

$$F \propto \beta_5 Q_{3z}^{\Gamma^2} Q_1^{R^2}$$

$$\beta_5 > 0$$

Zhang, Schmitt *et al.* Phys. Rev. B **98**, 081108(R), (2018)

[001] Epitaxial Strain Tuning: *From Charge- to Orbital-Order*

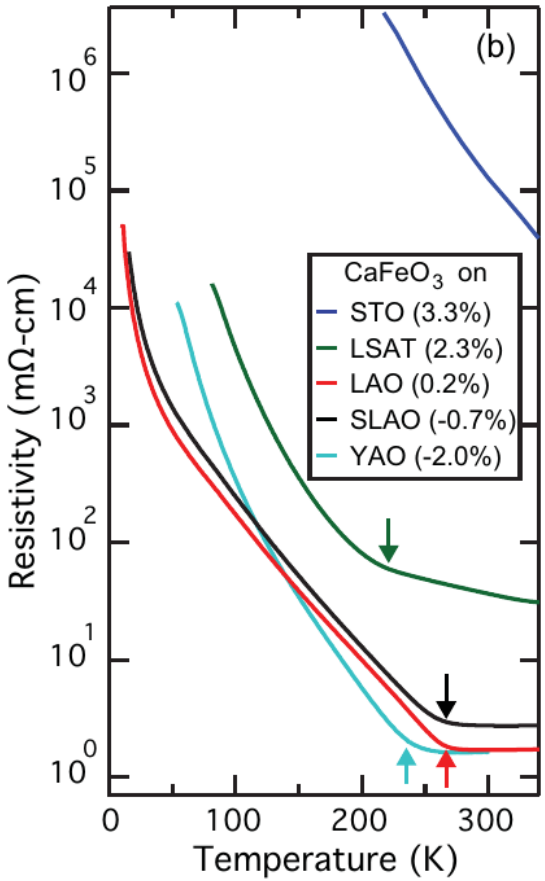


$$F \propto \beta_3 Q_{3z}^\Gamma$$

$$|\beta_3$$

$$F \propto$$

Experimental



Paul C. Rogge *et al* Phys. Rev. Materials **2**, 015002 (2018)

Zhang, Schmitt *et al.* Phys. Rev. B **98**, 081108(R), (2018)

Application III: [001] vs [111] Epitaxial Strain in $NdNiO_3$

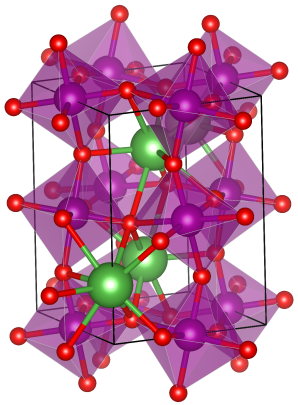
GS of $NdNiO_3$

GS

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

$+\ Q_1^{\mathbf{R}}$

$\rightarrow P2_1/n$



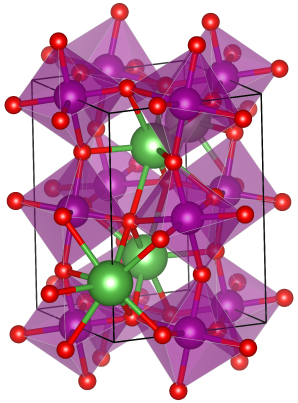
GS of $NdNiO_3$

GS

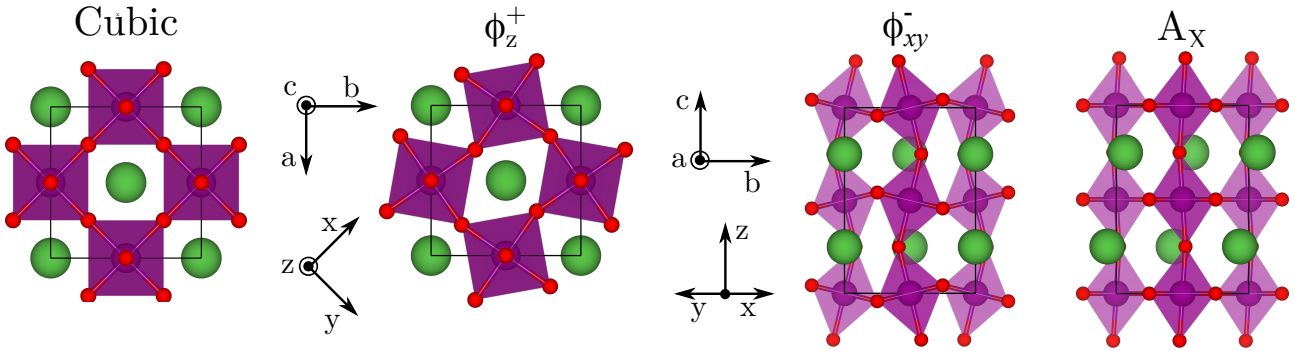
$Pnma\ a^-a^-c^+$

$+\ Q_1^{\mathbf{R}}$

$\rightarrow P2_1/n$



$T > 200K$ Metallic $Pnma$



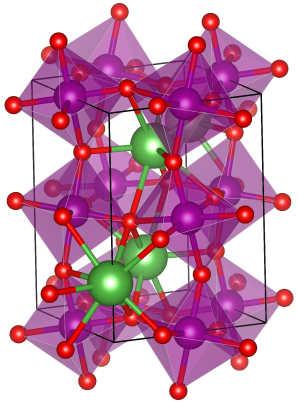
GS of $NdNiO_3$

GS

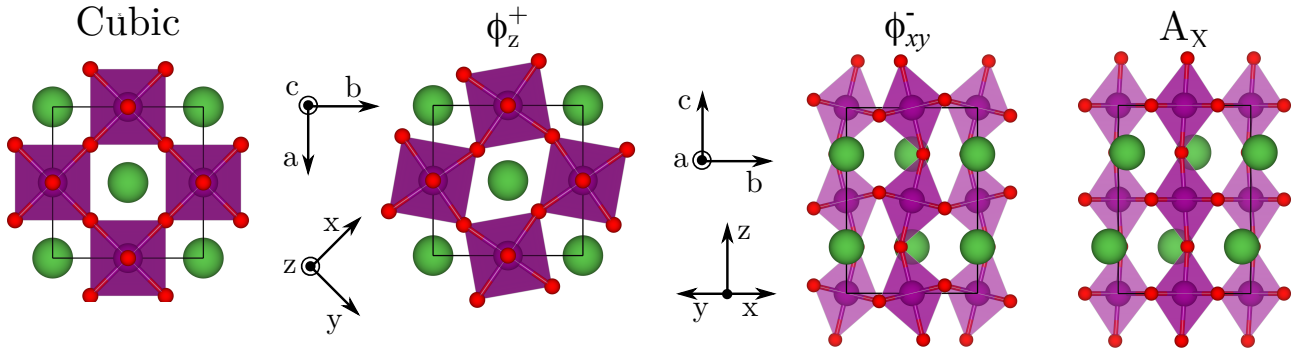
$Pnma\ a^-a^-c^+$

$+\ Q_1^{\mathbf{R}}$

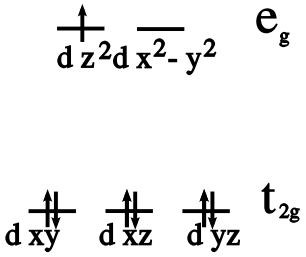
$\rightarrow P2_1/n$



$T > 200K$ Metallic $Pnma$



$\mathbf{Ni^{3+} = d^7}$



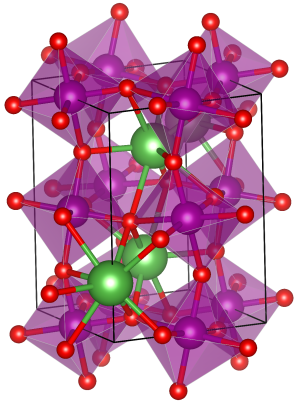
GS of $NdNiO_3$

GS

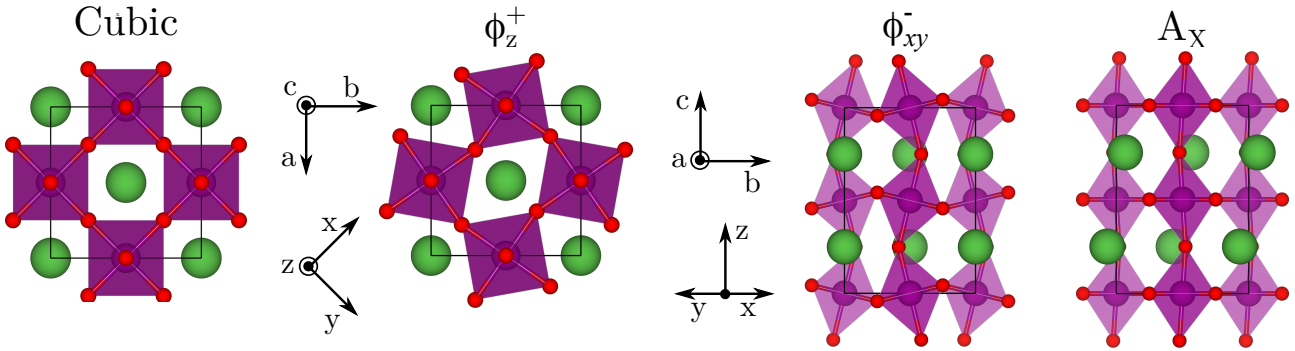
$Pnma\ a^-a^-c^+$

$+\ Q_1^{\mathbf{R}}$

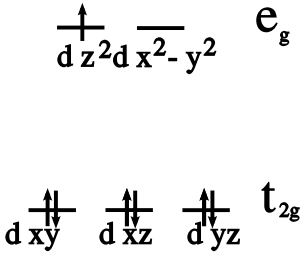
$\rightarrow P2_1/n$



$T > 200K$ Metallic $Pnma$



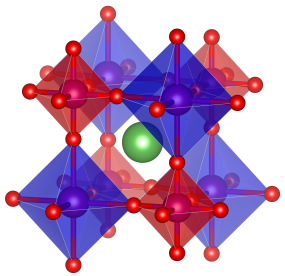
$\mathbf{Ni^{3+} = d^7}$



$T < T_{MIT} \approxeq 200K$ Ins. $P2_1/n$

AFM $T < T_N \approxeq 200$K

$Q_1^{\mathbf{R}}$

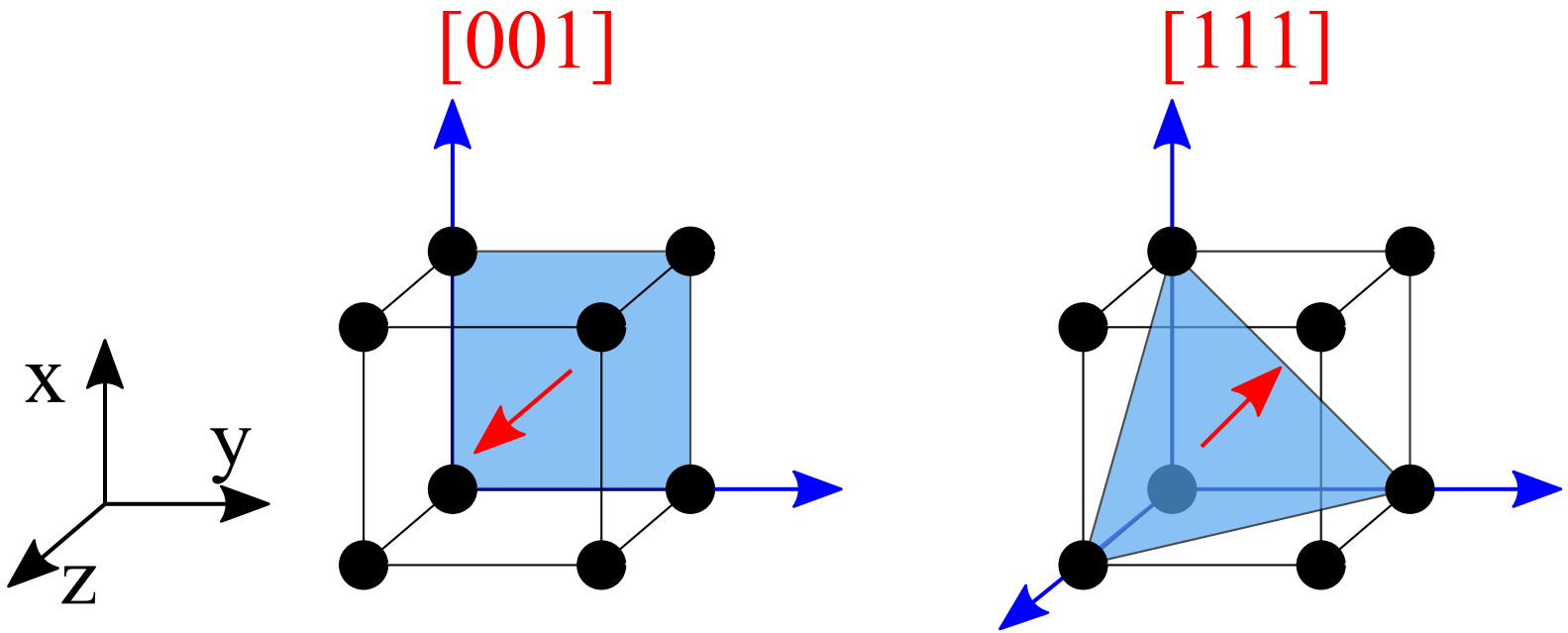


GS of $NdNiO_3$

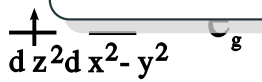
GS

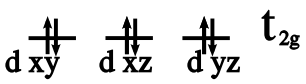
Pnm

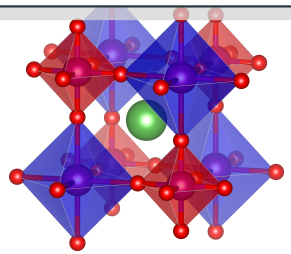
Effect of [001] vs [111] epitaxial strain?



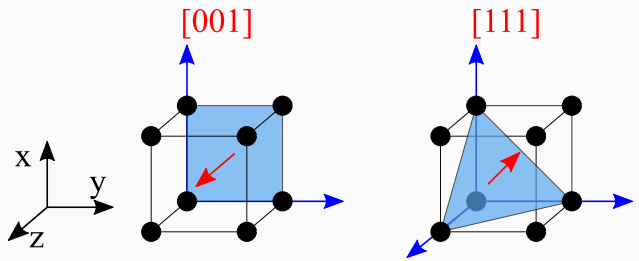
Ni

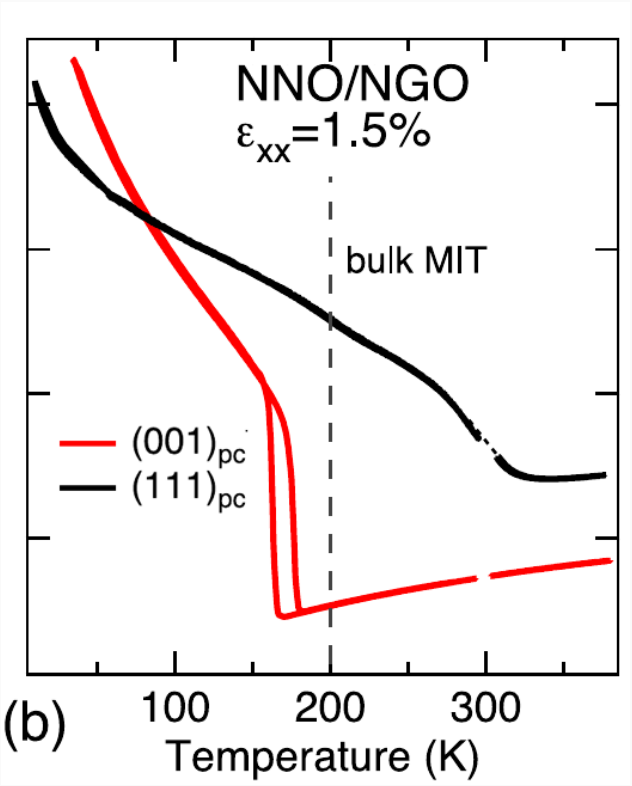






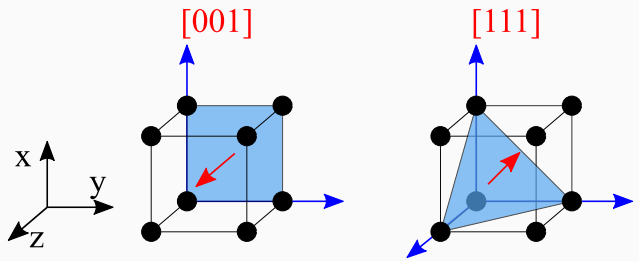
[001] vs. [111] Epitaxial Strain

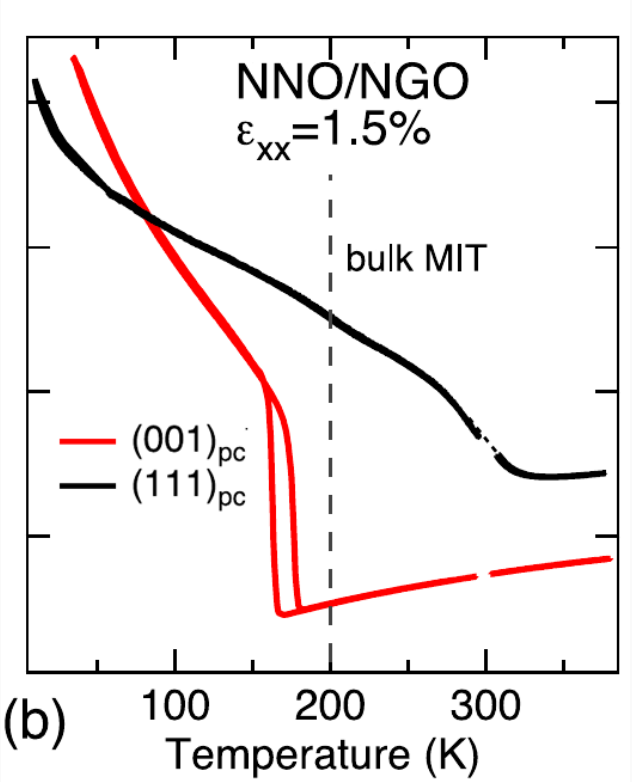


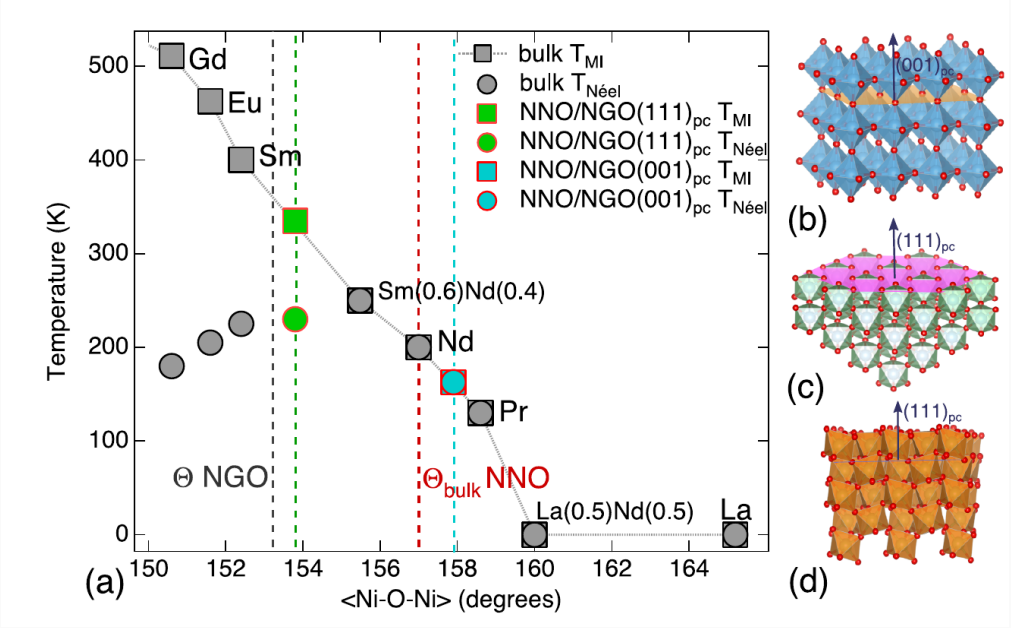


Catalano, S., et al. APL materials **3.6** (2015)

[001] vs. [111] Epitaxial Strain

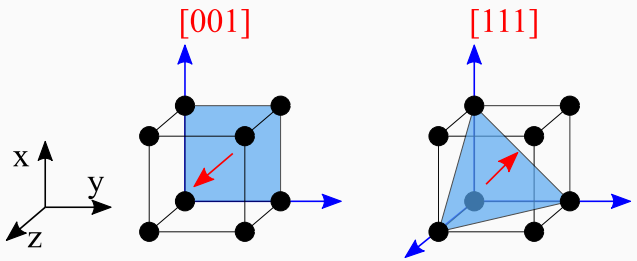


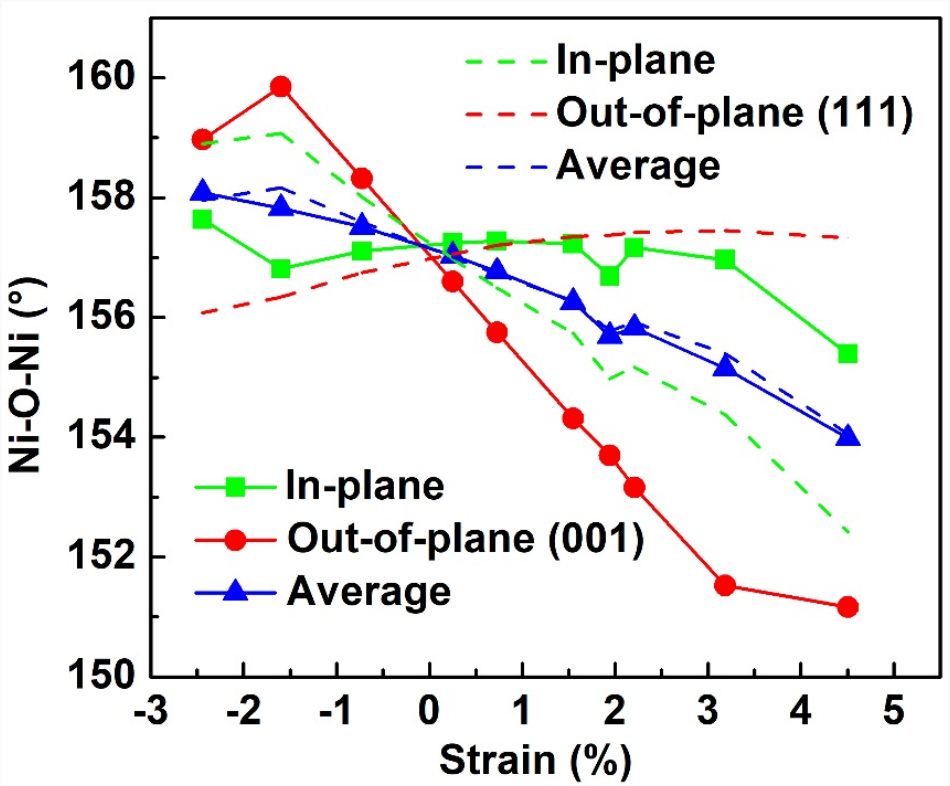


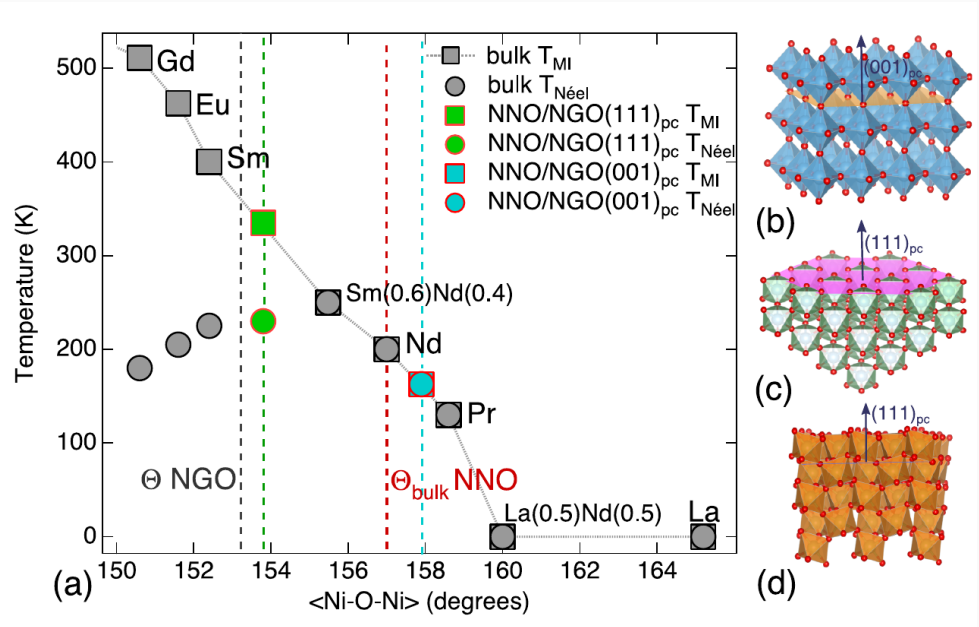


Catalano, S., et al. APL materials **3.6** (2015)

[001] vs. [111] Epitaxial Strain



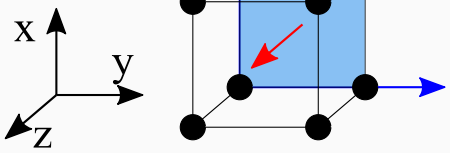




Catalano, S., et al. APL materials **3.6** (2015)

[001] vs. [111] Epitaxial Strain

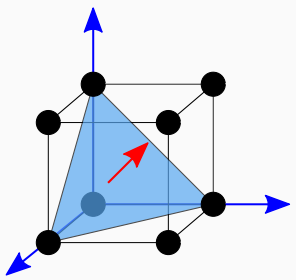
[001]



$Q_1^\Gamma \neq 0$ & $Q_{3z}^\Gamma \neq 0$

$Q_{4x,y,z}^\Gamma = 0$

[111]



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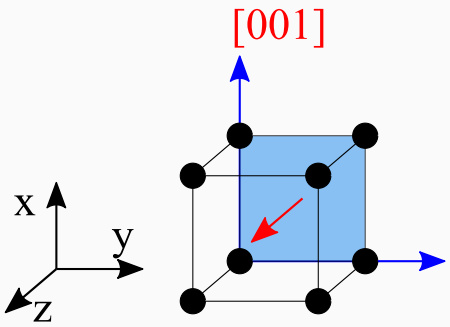

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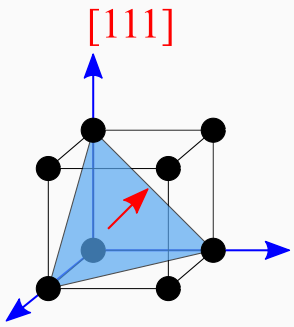

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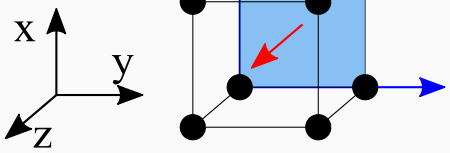
$Q_{3z}^\Gamma = 0$

	NNO /NGO$[001]_{pc}$	NNO /NGO$[111]_{pc}$
Q_1^Γ	0.014	0.014
Q_{3z}^Γ	-0.029	0.000
Q_{4z}^Γ	0.009	0.026
$Q_{4x,y}^\Gamma$	0.000	0.016

[001] vs. [111] Epitaxial Strain

[001]



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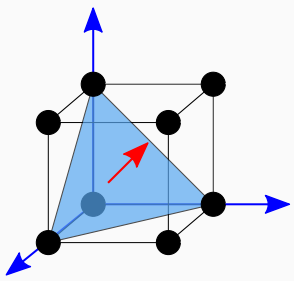

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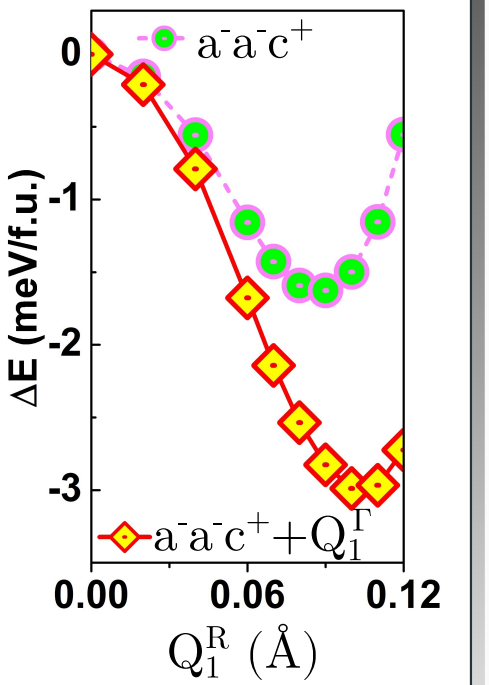
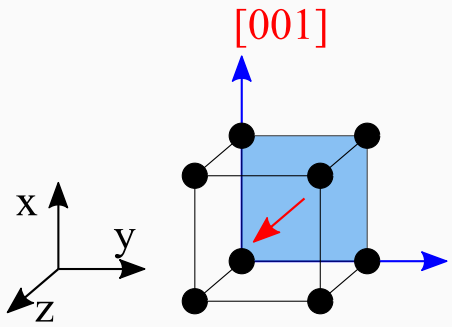


[001] vs. [111] Epitaxial Strain



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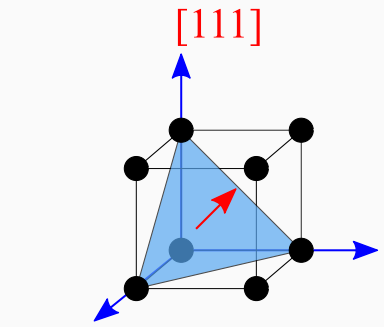

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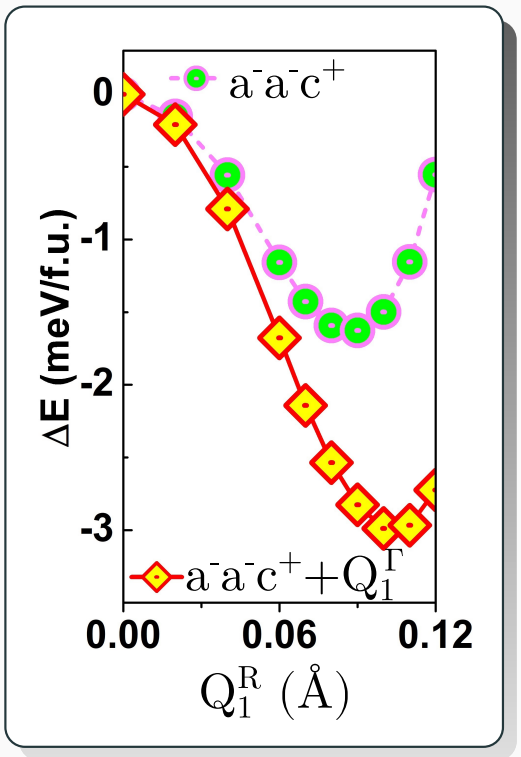
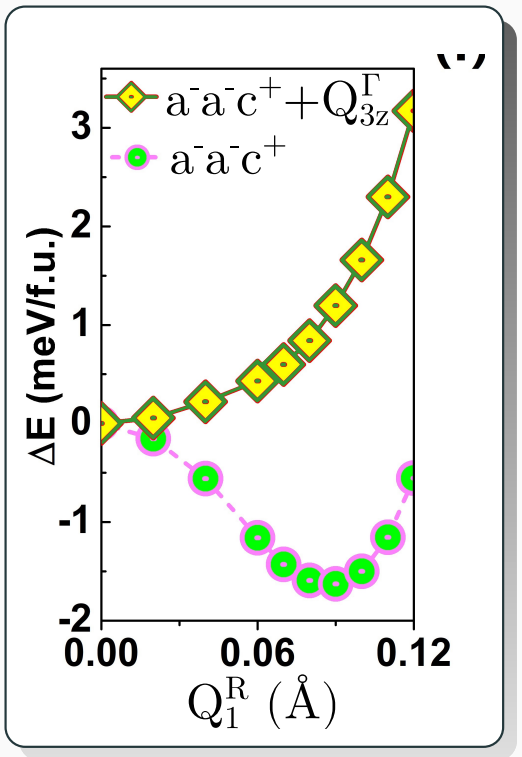
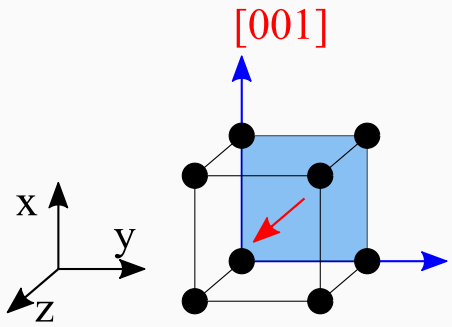




[001] vs. [111] Epitaxial Strain



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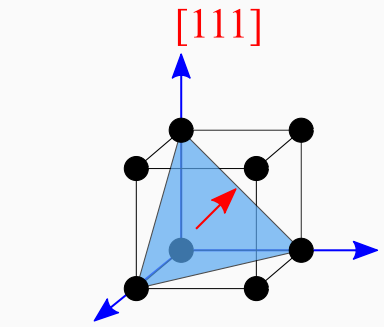

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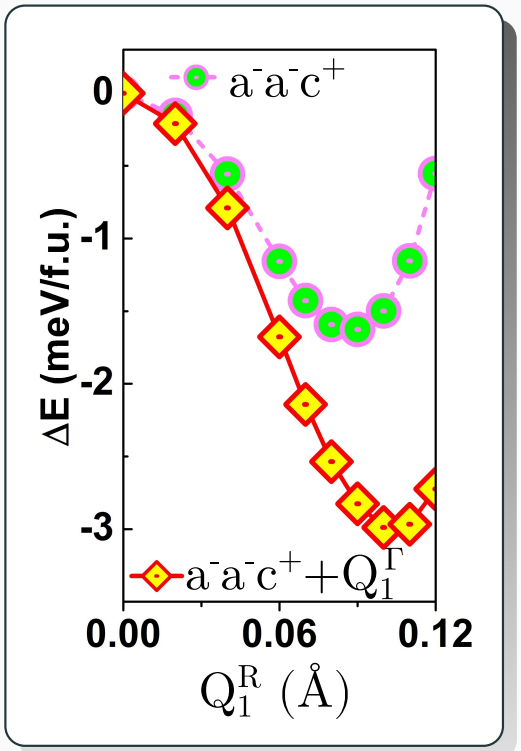
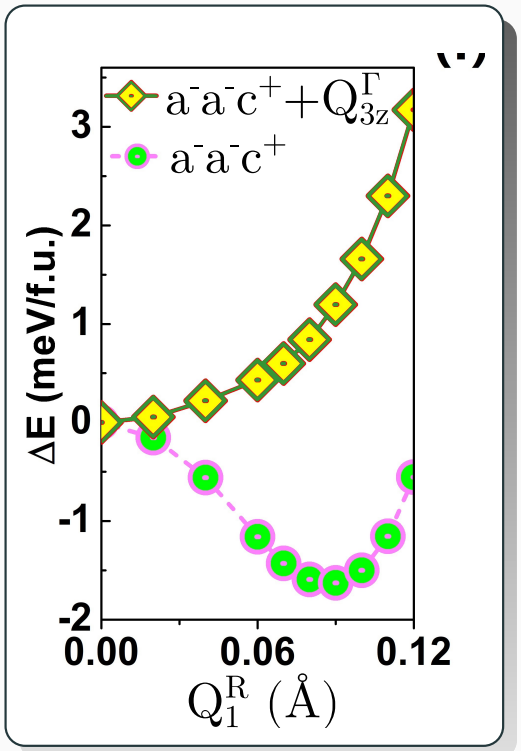
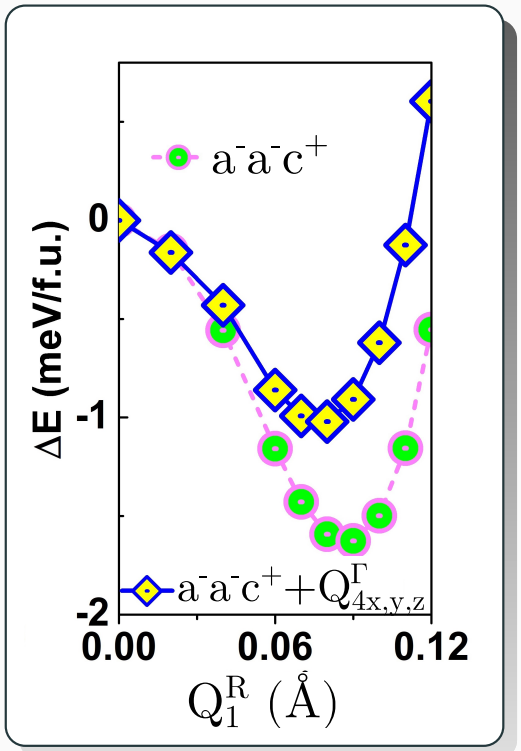
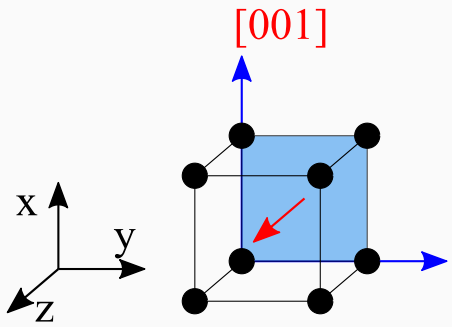


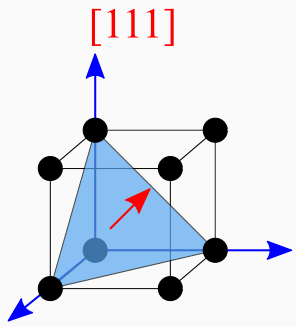




[001] vs. [111] Epitaxial Strain



$Q_1^\Gamma \neq 0$ & $Q_{3z}^\Gamma \neq 0$



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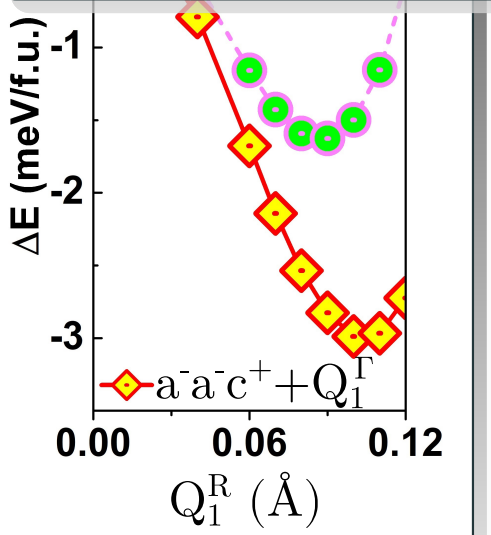
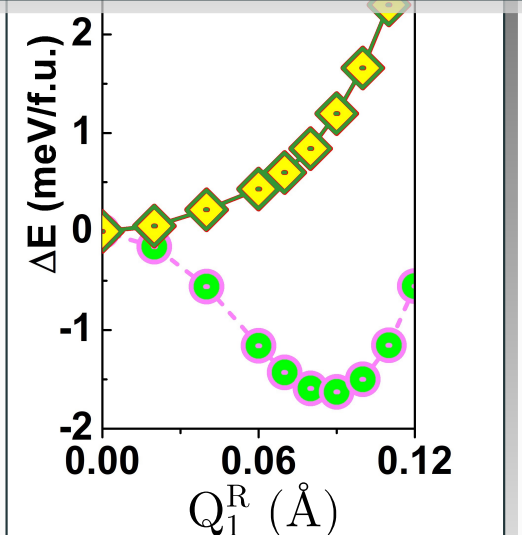
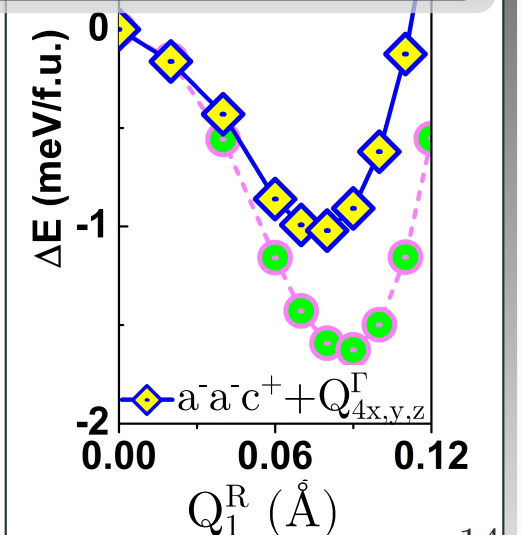
Tetragonal Strain Q_{3z}^Γ hinders MIT

Q_{3z}^Γ competes with Q_1^Γ and increased rotations

On NGO [111] $Q_{3z}^\Gamma = 0$ while Q_ϕ and Q_1^Γ same as on [001] NGO



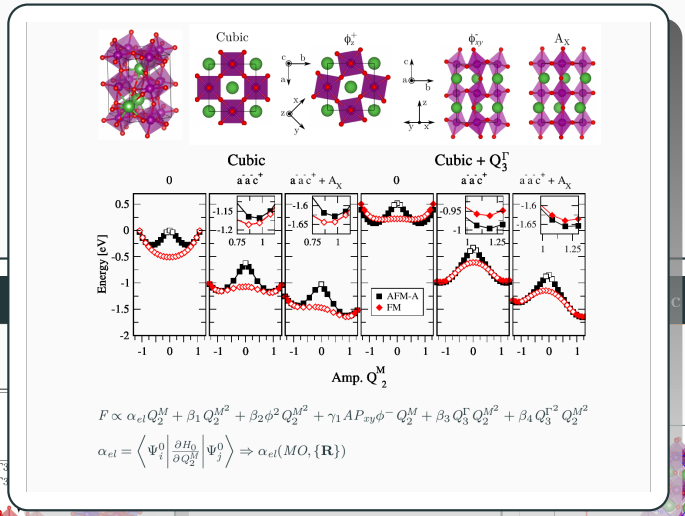


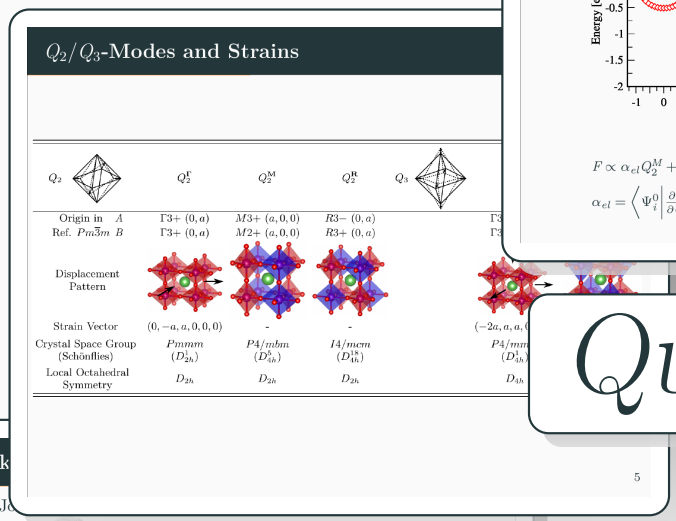


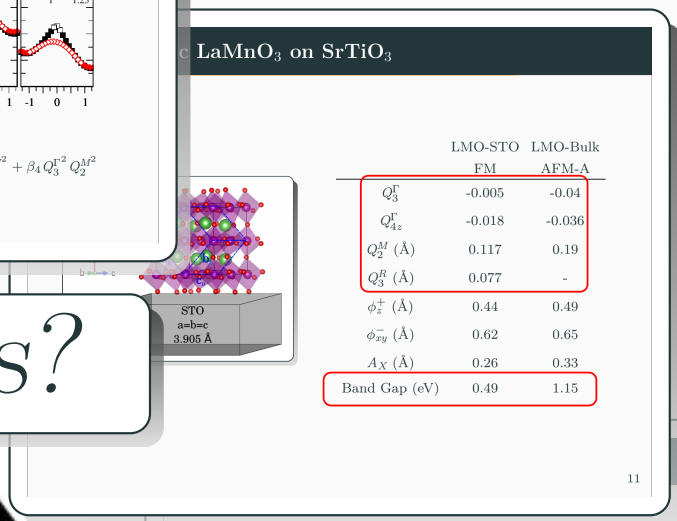
Conclusions

- Canonical Jahn-Teller Distortion Notations $Q_{i\alpha}^{\vec{q}}$ for anaylizing Perovskite Materials
  → Schmitt, M. M., et al, arXiv:1909.06287 (2019)
- Tetragonal Strain $Q_{3\alpha}^{\Gamma}$ cooperative with orbital-ordered (Jahn-Teller distorted) phases in e_g^1 perovskites
- Tetragonal Strain $Q_{3\alpha}^{\Gamma}$ *anti*-cooperative with charge-ordered (Q_1^R-distorted) phases in e_g^1 perovskites
- Strain and Rotation state in thin film can be engineered by choice of substrate:
  → Space-Group of Substrate (Rotations/No-Rotations)
  → Surface of Substrate [001],[011],[111]..
  → Lattice Mismatch between substrate and thin film

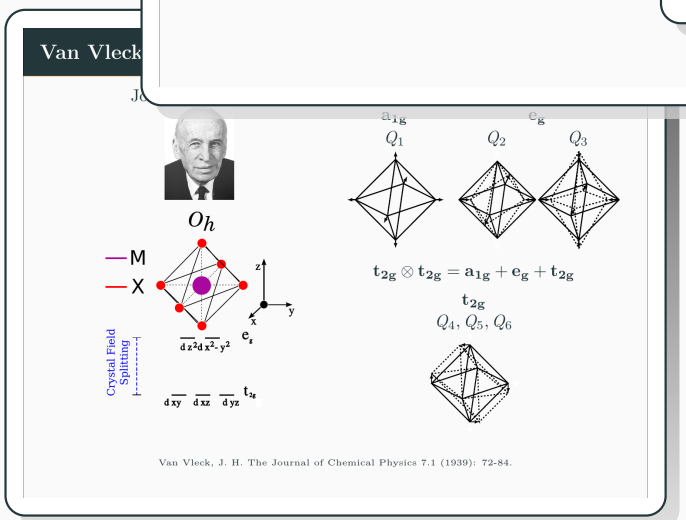
Thank you for your attention!

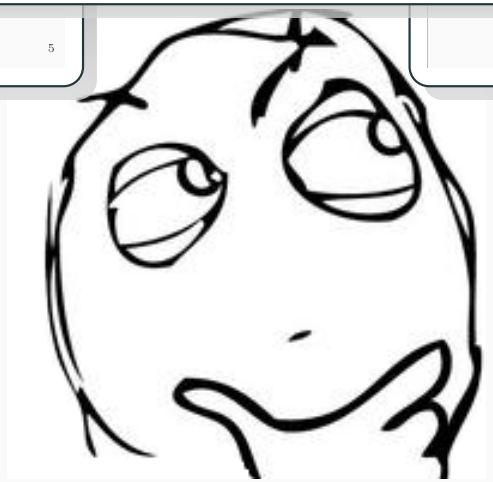


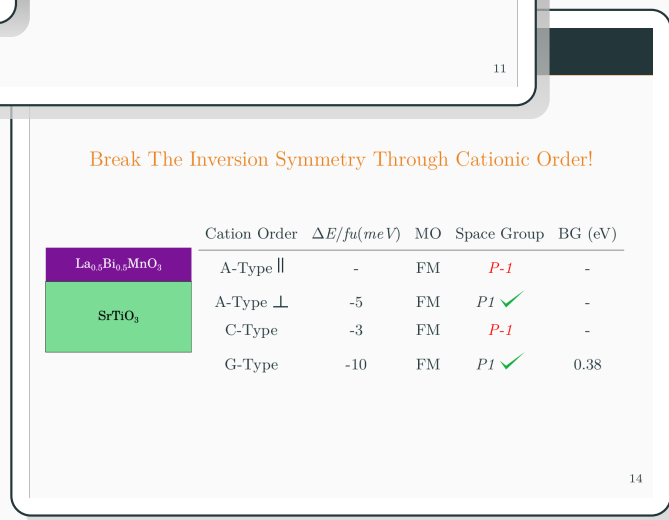




Questions?







Ferromagnetic $LaMnO_3$ on $SrTiO_3$

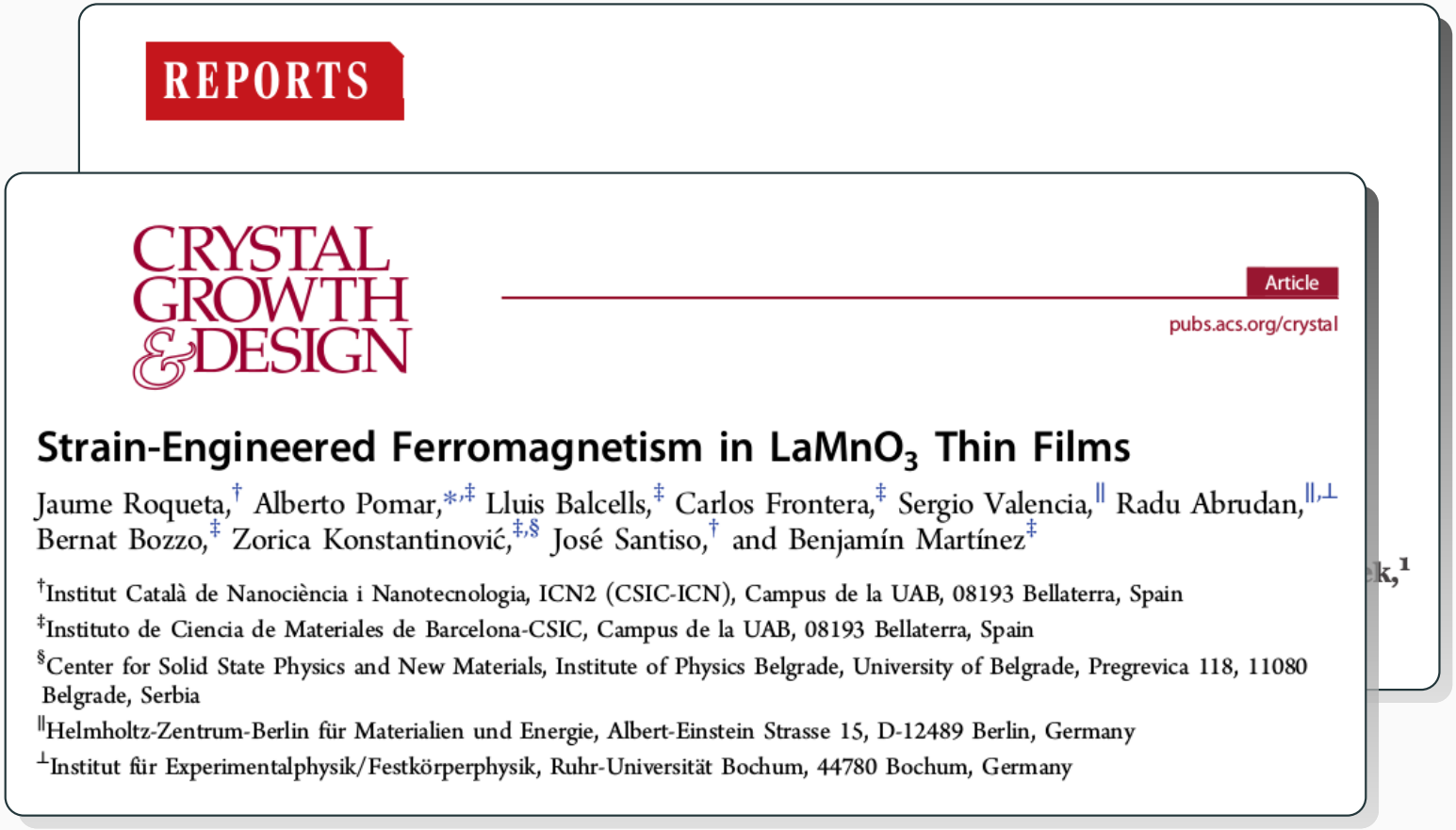
REPORTS

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

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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

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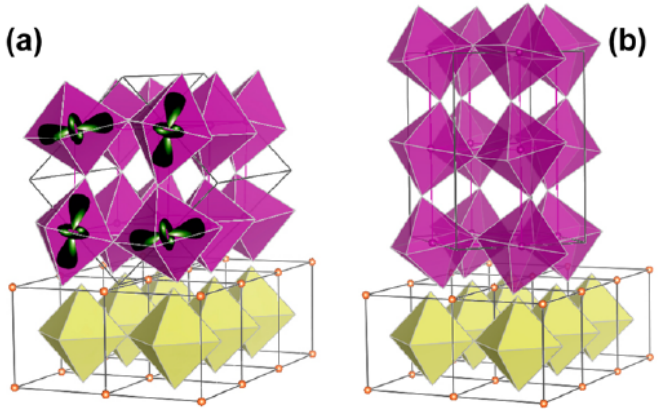

Roqueta J.,*et al.* Cryst. Growth Des. **15.11** (2015)

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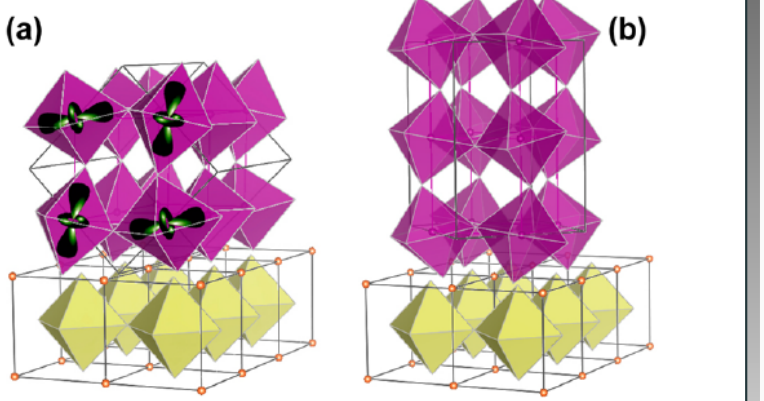

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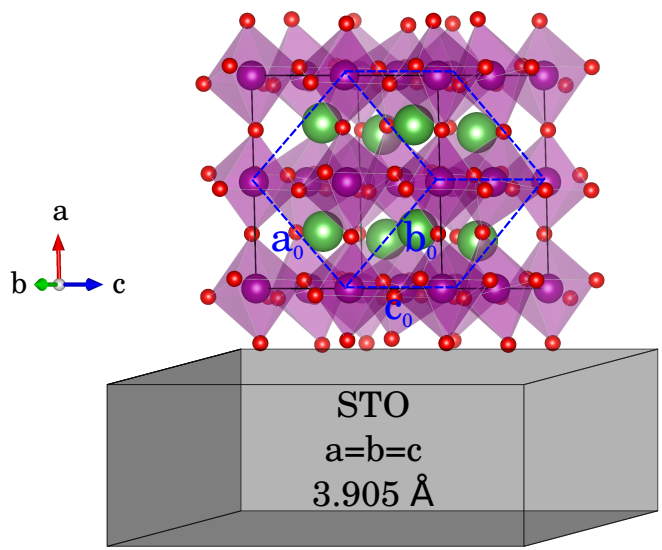

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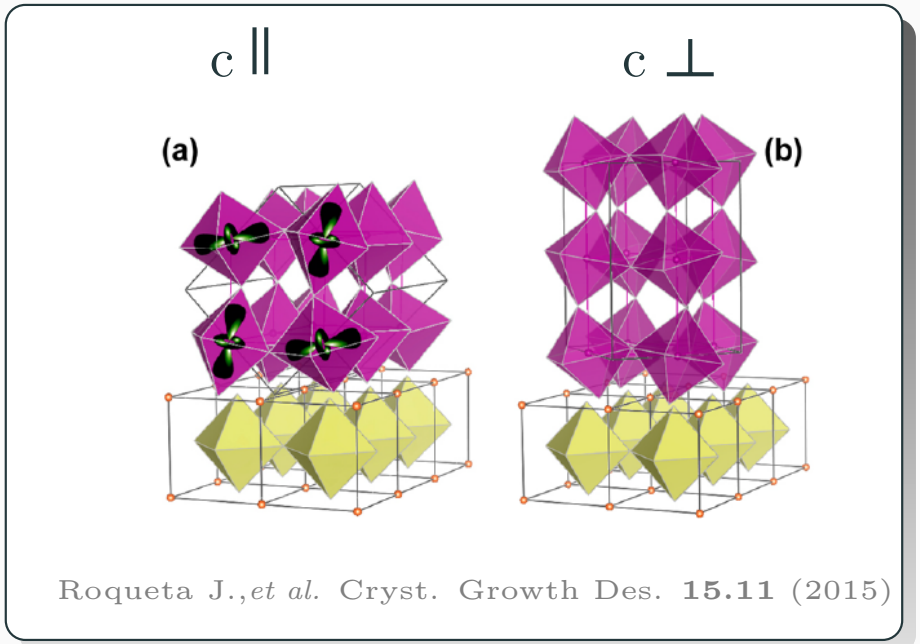

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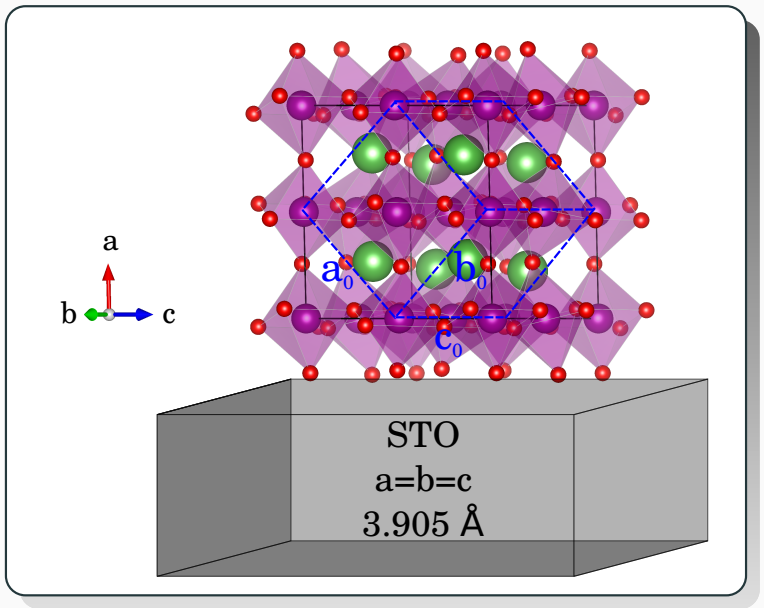
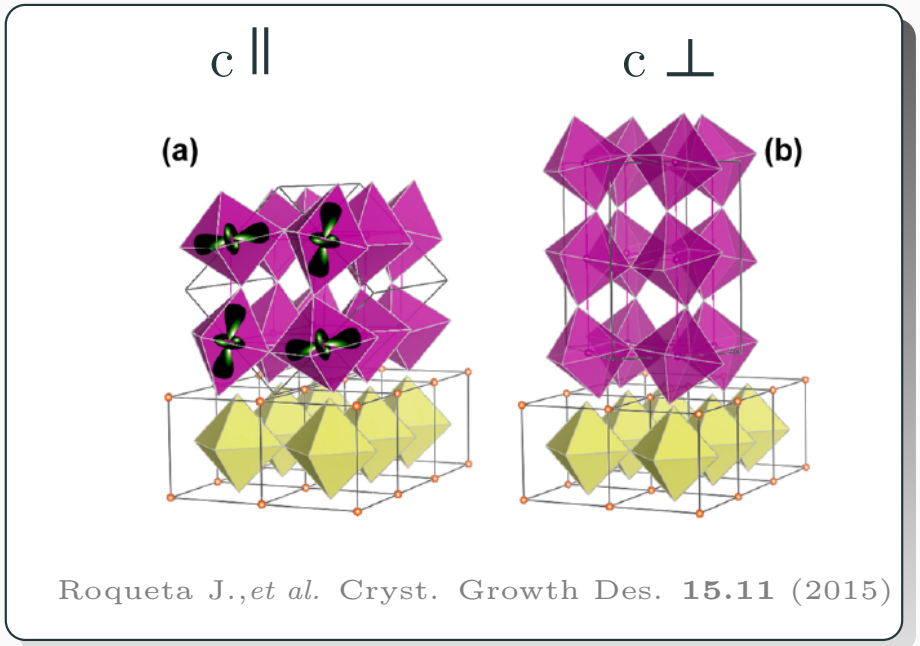


	LMO-STO *P-1* FM	LMO-Bulk *Pnma* AFM-A
Q_3^Γ	-0.005	-0.04
Q_{4z}^Γ	-0.018	-0.036
Q_2^M (Å)	0.117	0.19
Q_3^R (Å)	0.077	-
ϕ_z^+ (Å)	0.44	0.49
ϕ_{xy}^- (Å)	0.62	0.65
A_X (Å)	0.26	0.33
Band Gap (eV)	0.49	1.15

Ferromagnetic $LaMnO_3$ on $SrTiO_3$



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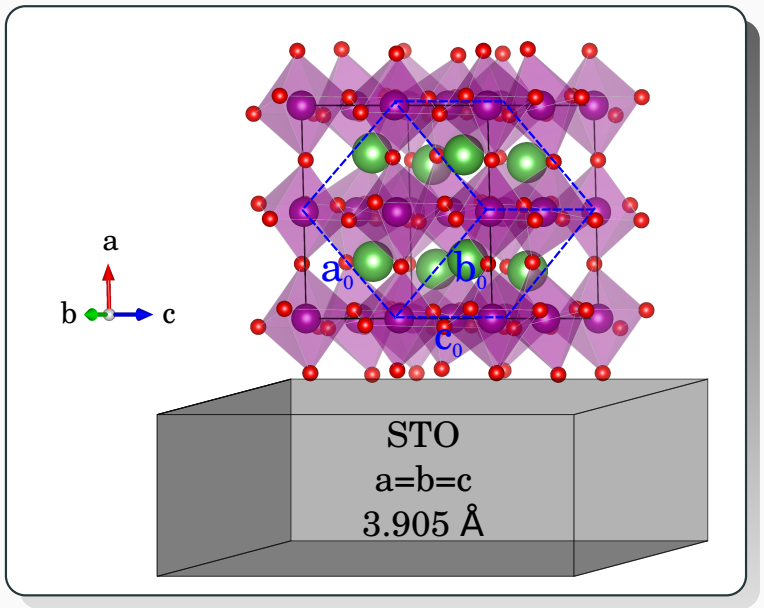

	LMO-STO	LMO-Bulk
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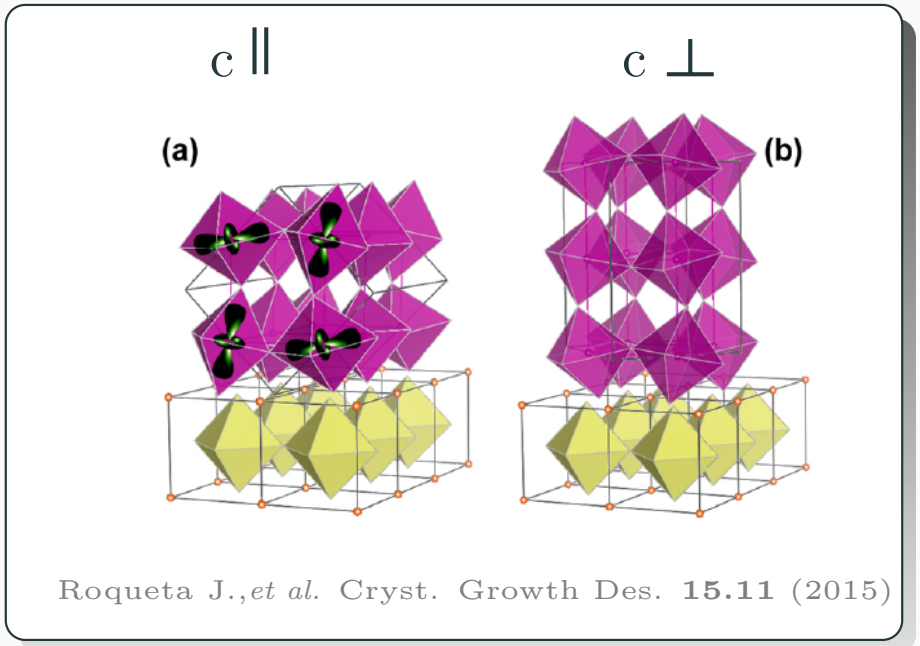
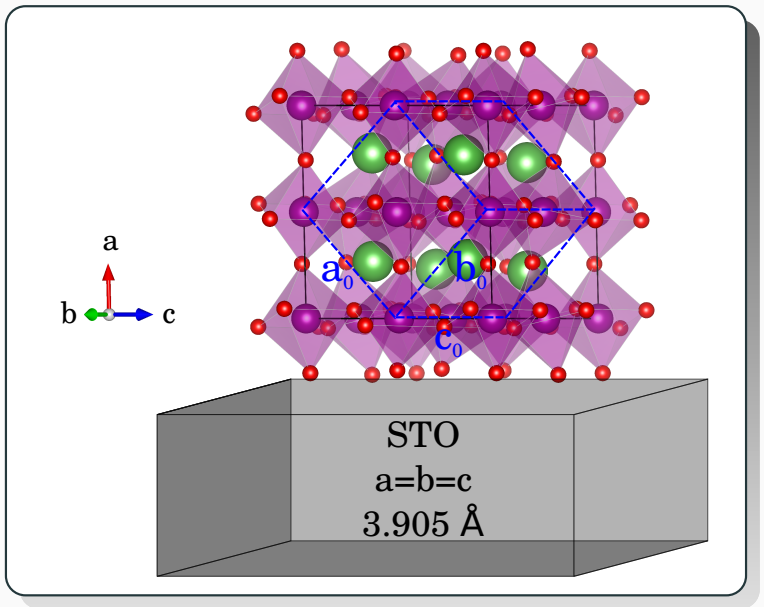
A_X (Å)	0.26	0.33
Band Gap (eV)	0.49	1.15

Ferromagnetic $LaMnO_3$ on $SrTiO_3$

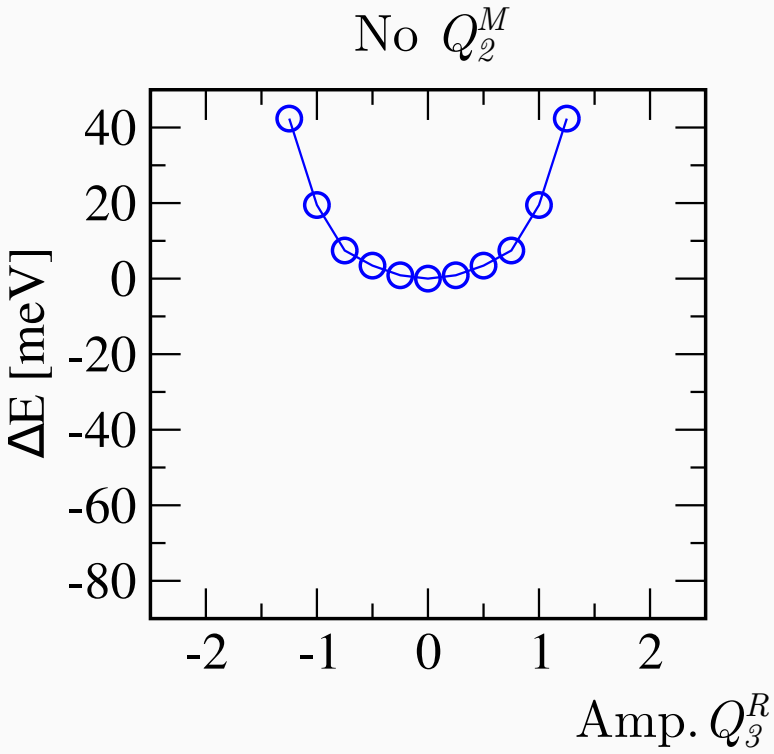


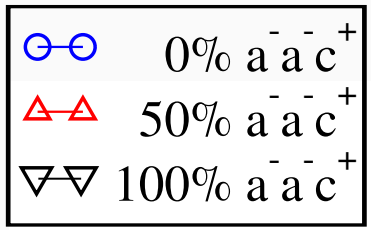
Roqueta J.,*et al.* Cryst. Growth Des. **15.11** (2015)



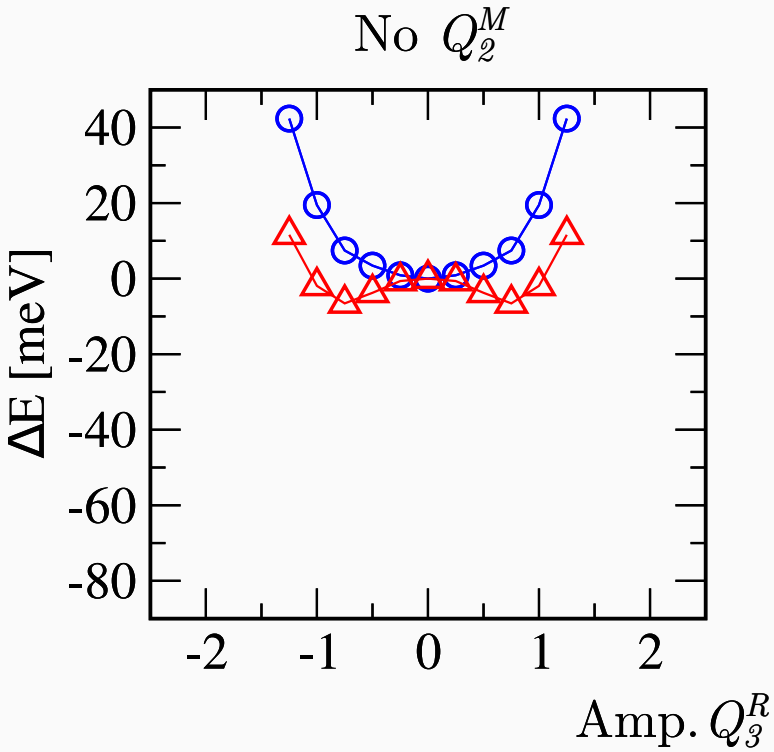
	LMO-STO *P-1* FM	LMO-Bulk *Pnma* AFM-A
Q_3^Γ	-0.005	-0.04
Q_{4z}^Γ	-0.018	-0.036
Q_2^M (Å)	0.117	0.19
Q_3^R (Å)	0.077	-
ϕ_z^+ (Å)	0.44	0.49
ϕ_{xy}^- (Å)	0.62	0.65
A_X (Å)	0.26	0.33
Band Gap (eV)	0.49	1.15

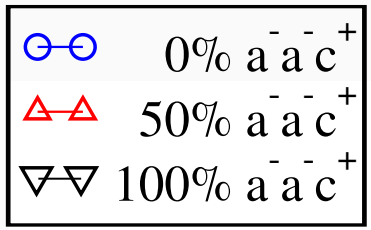
Q_3^R JTD



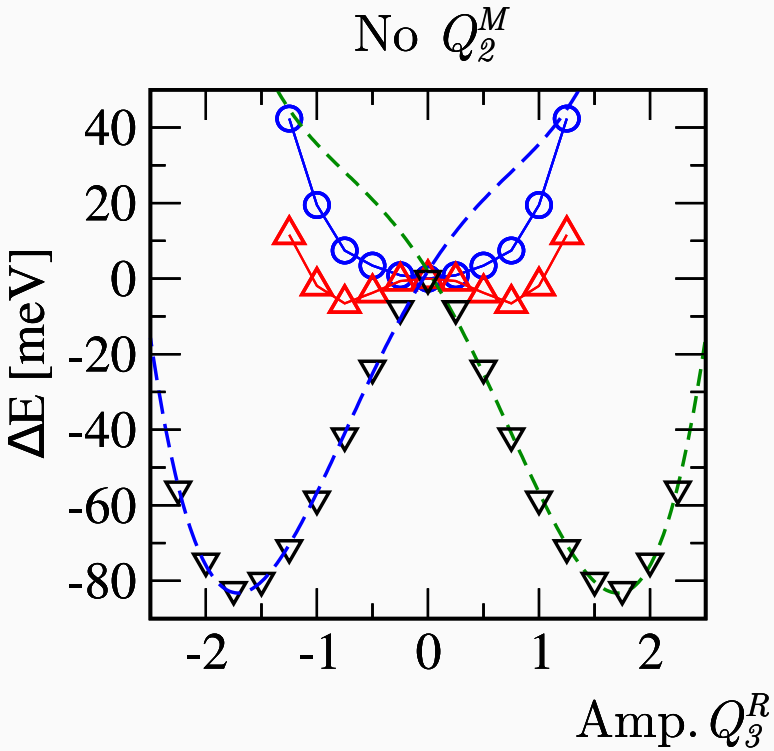


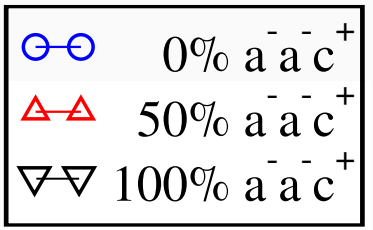
Q_3^R JTD



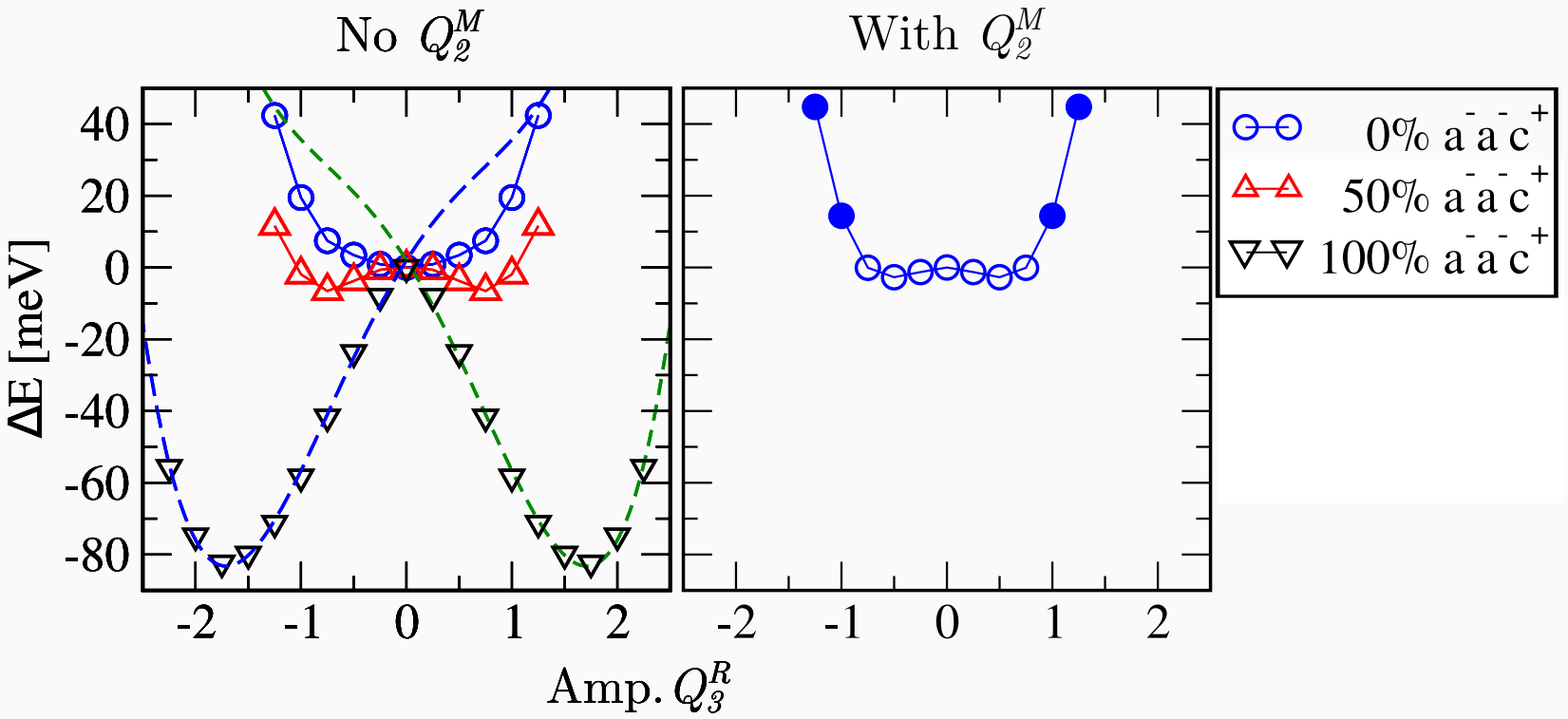


Q_3^R JTD

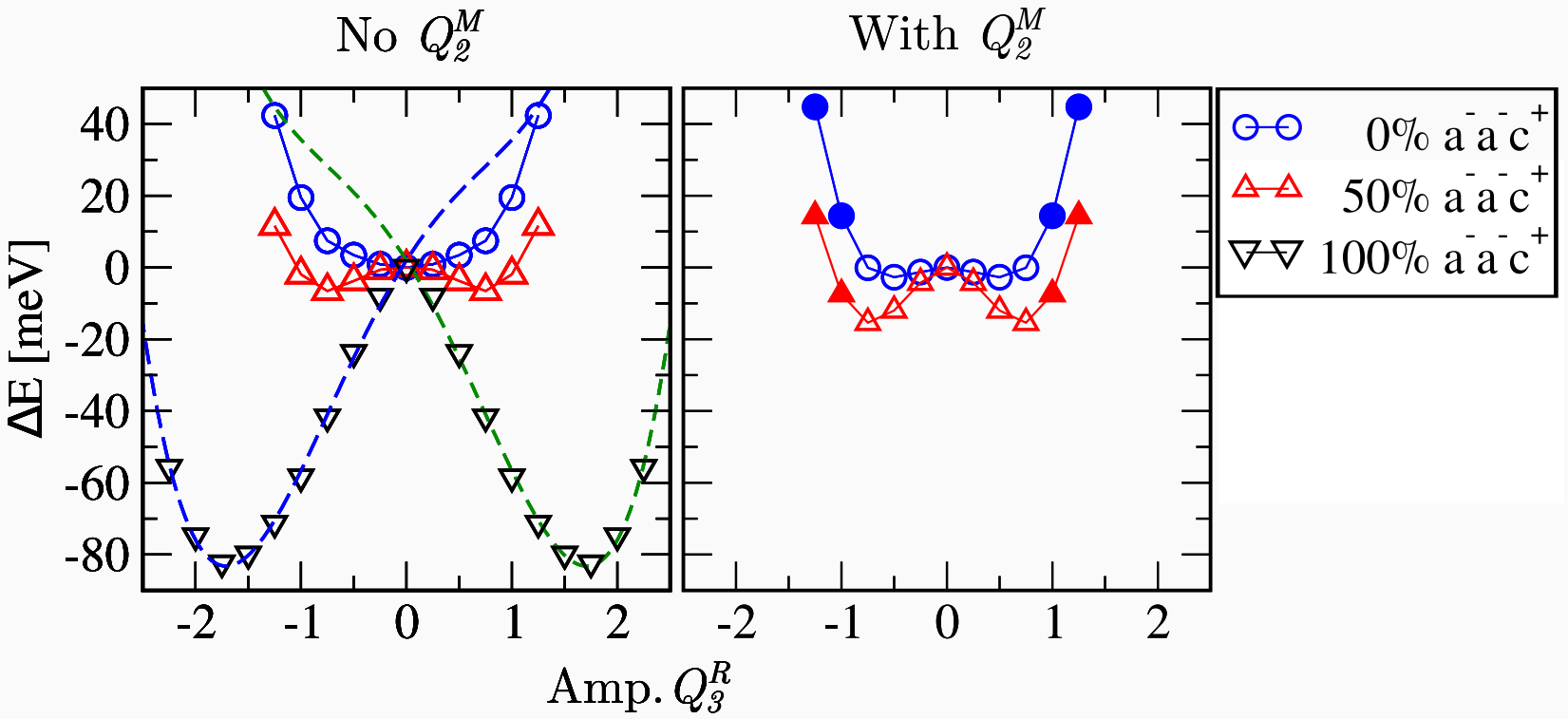




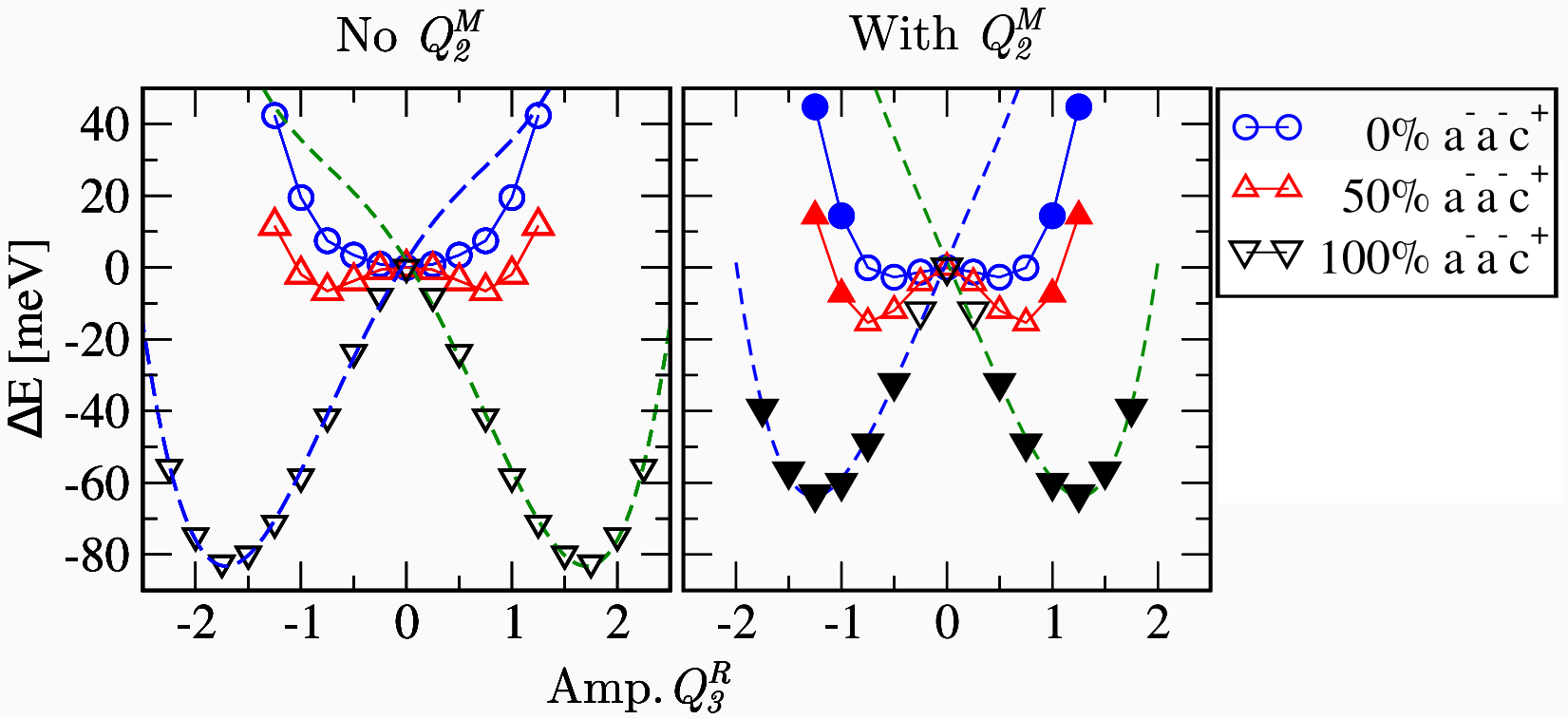
Q_3^R JTD


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
0% a⁻a⁻c⁺
50% a⁻a⁻c⁺
100% a⁻a⁻c⁺

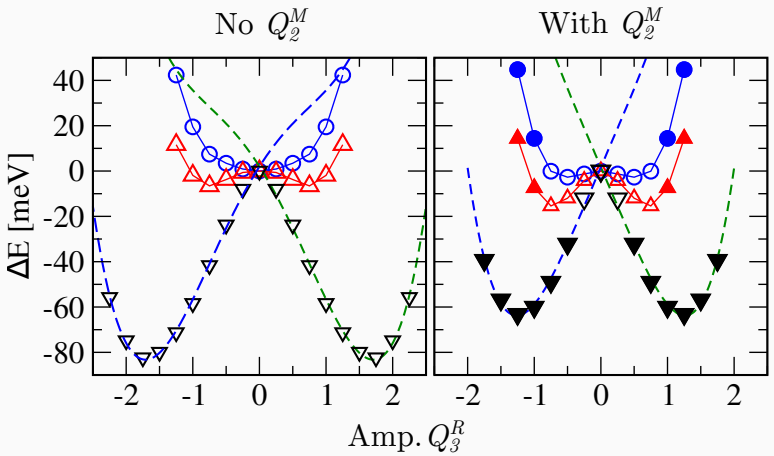
Q_3^R JTD

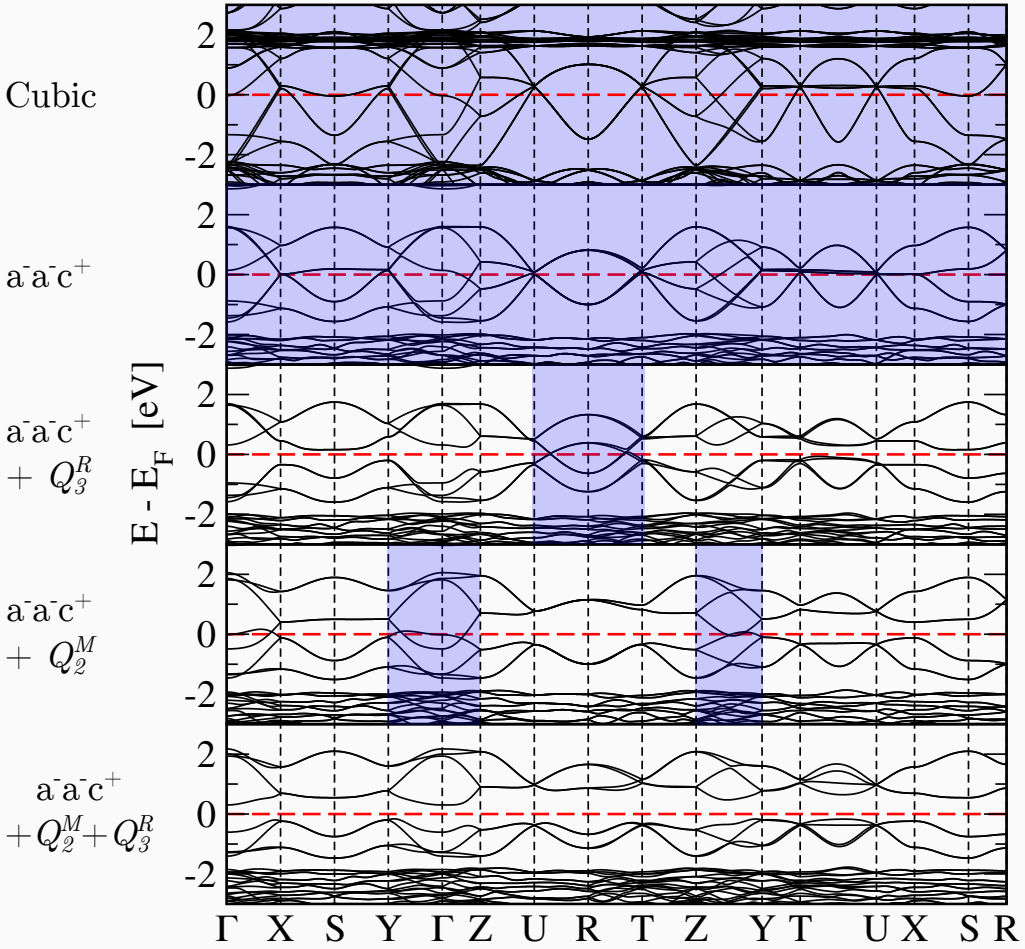

No Q_2^M
With Q_2^M
ΔE [meV]
40
20
0
-20
-40
-60
-80
-2
-1
0
1
2
Amp. Q_3^R
0% a⁻a⁻c⁺
50% a⁻a⁻c⁺
100% a⁻a⁻c⁺

Q_3^R JTD

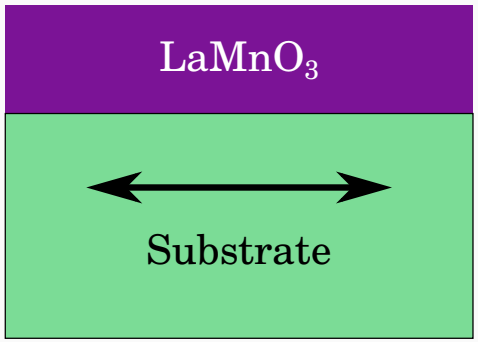

No Q_2^M
With Q_2^M
ΔE [meV]
40
20
0
-20
-40
-60
-80
-2
-1
0
1
2
Amp. Q_3^R
0% a⁻a⁻c⁺
50% a⁻a⁻c⁺
100% a⁻a⁻c⁺

Q_3^R JTD

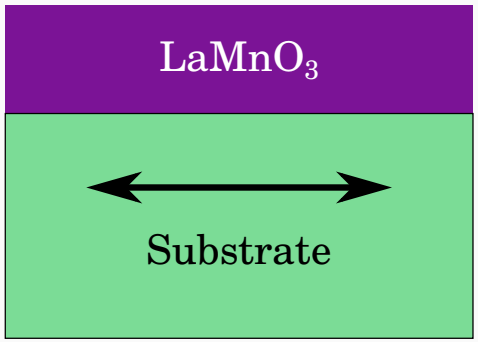

No Q_2^M
With Q_2^M
ΔE [meV]
40
20
0
-20
-40
-60
-80
-2
-1
0
1
2
Amp. Q_3^R

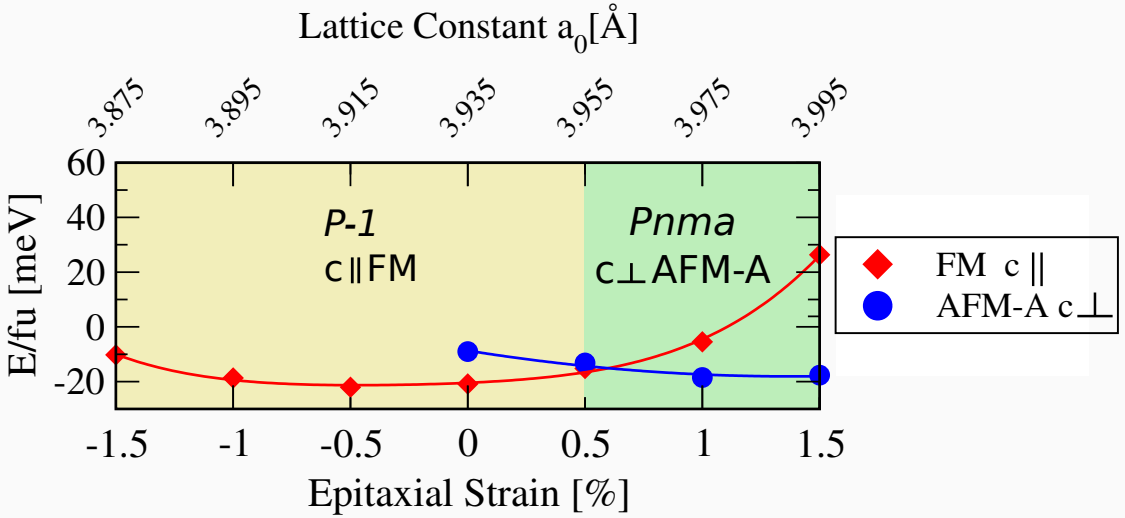

Cubic
a⁻a⁻c⁺
a⁻a⁻c⁺ + Q_3^R
a⁻a⁻c⁺ + Q_2^M
a⁻a⁻c⁺ + Q_2^M + Q_3^R
E - E$_F$ [eV]
2
0
-2
Γ X S Y Γ Z U R T Z Y T U X S R

Strain Engineering in $LaMnO_3$

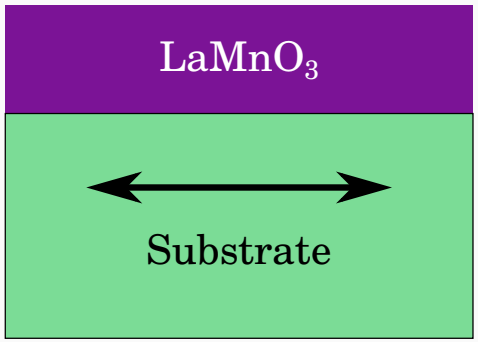


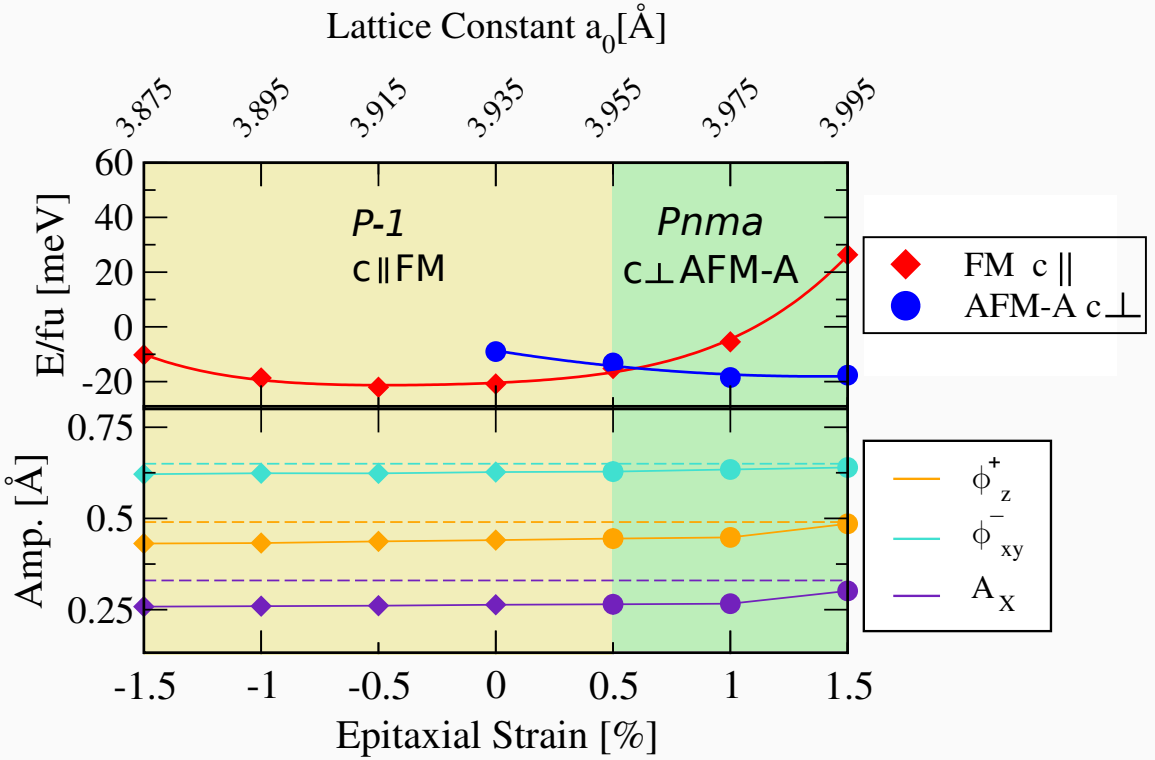
Strain Engineering in $LaMnO_3$



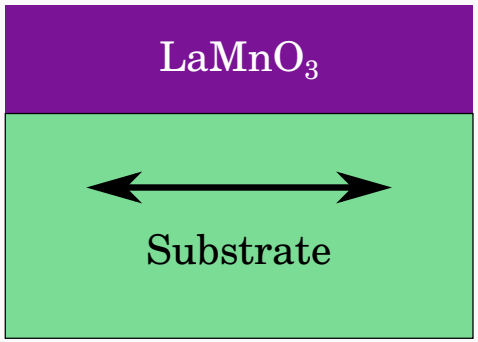


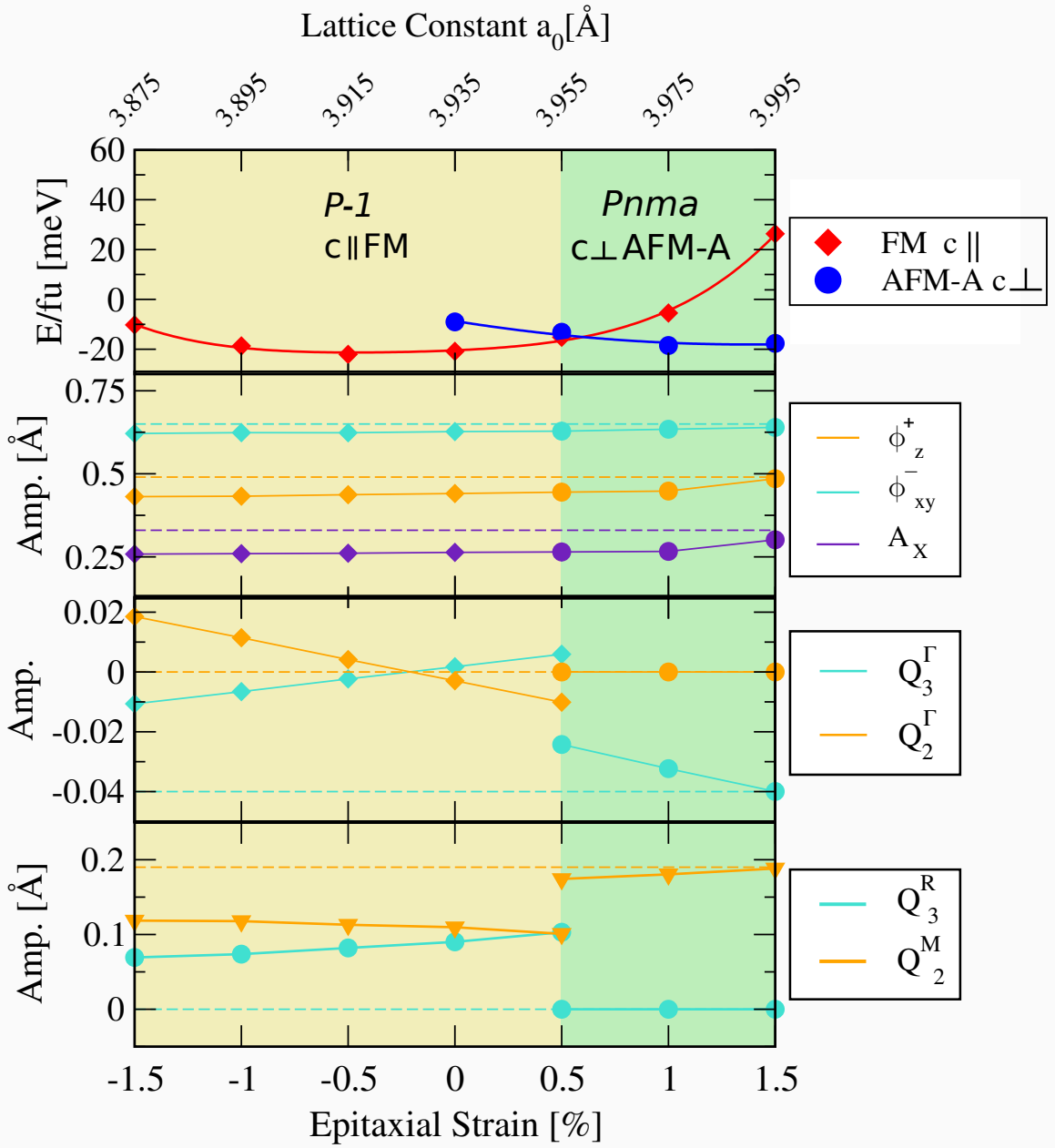
Strain Engineering in $LaMnO_3$



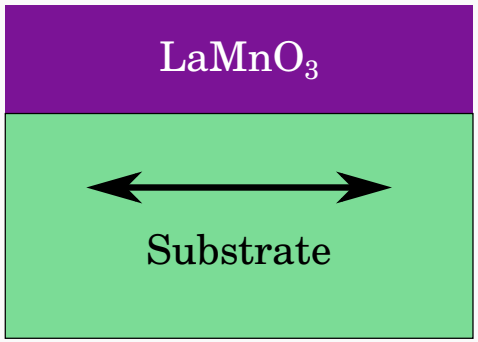


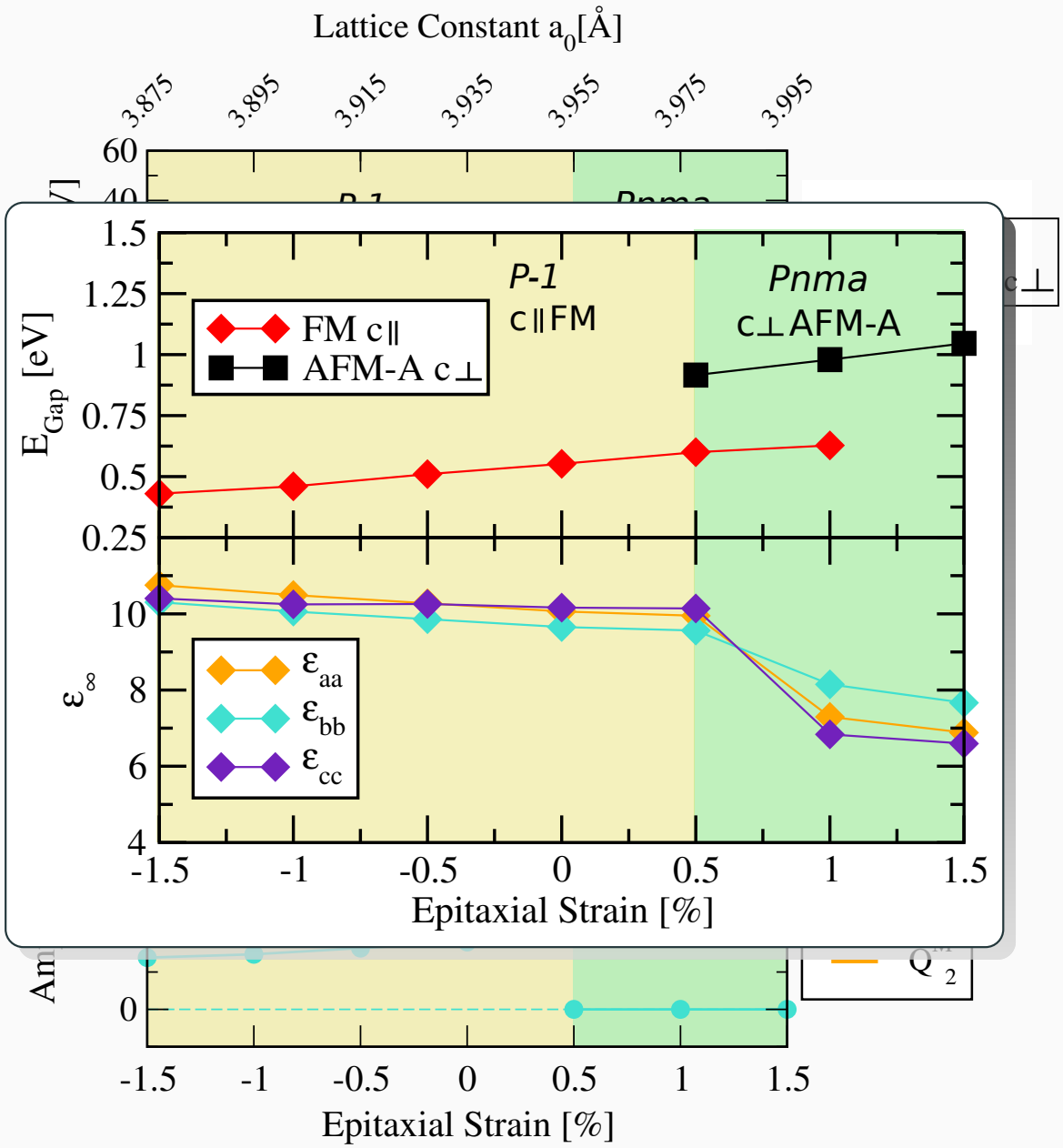
Strain Engineering in $LaMnO_3$



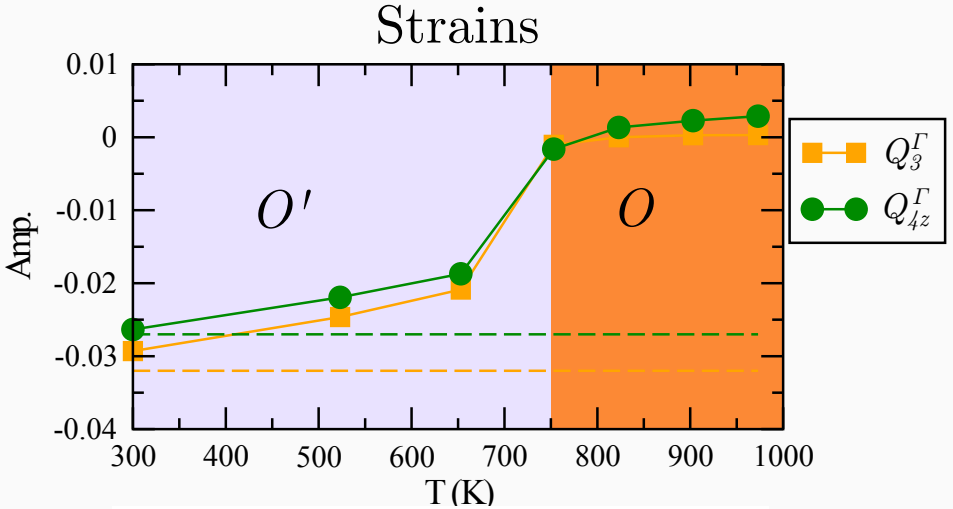


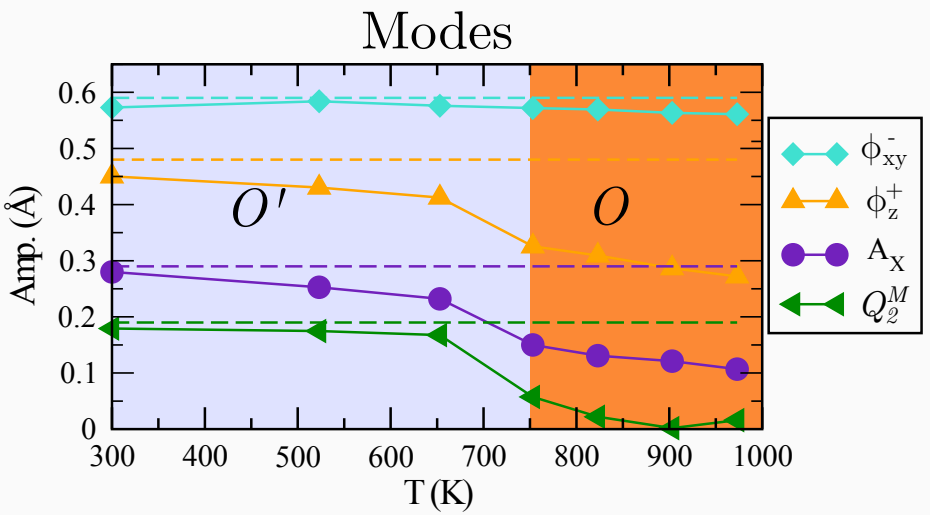
Strain Engineering in $LaMnO_3$

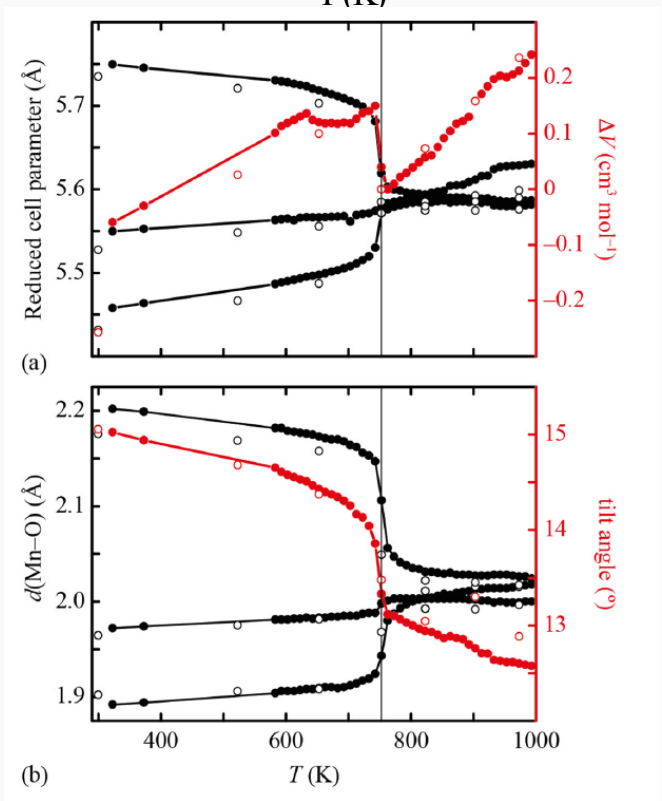




Modes and Strains across T_{MIT} $LaMnO_3$







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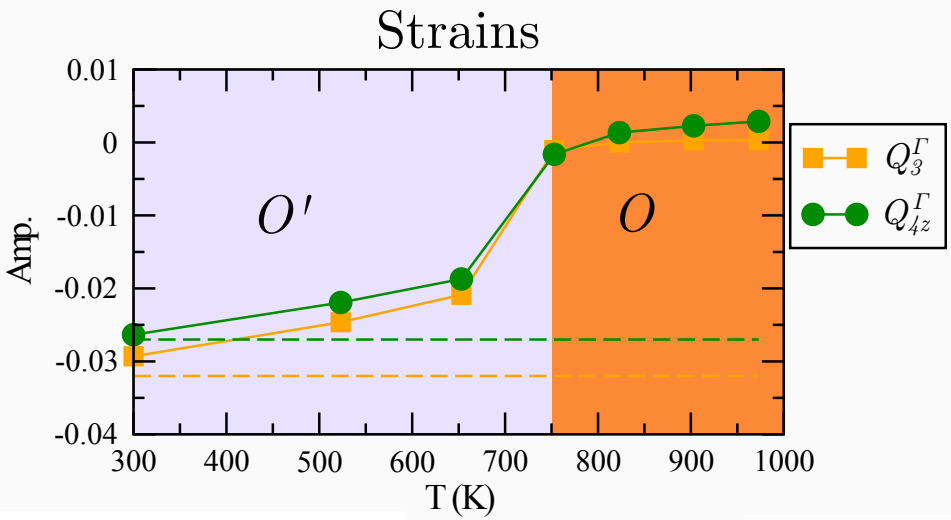
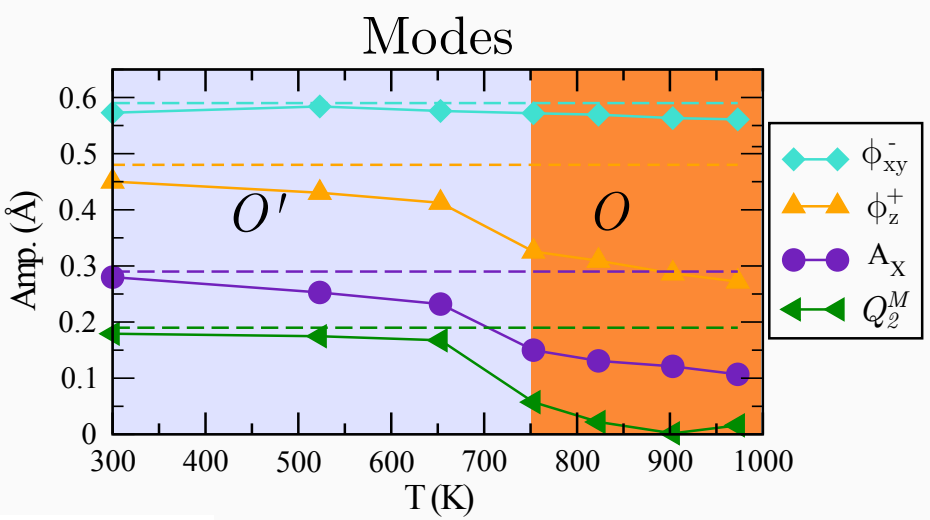
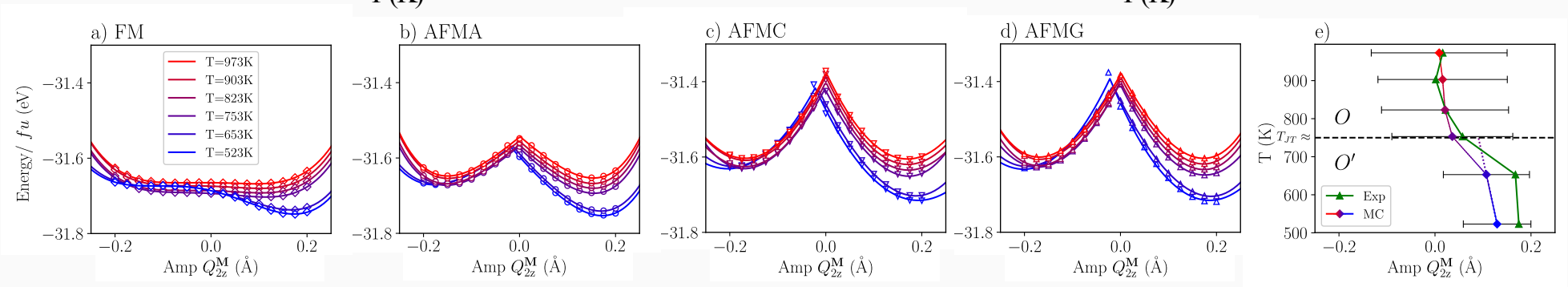
Modes and Strains across T_{MIT} $LaMnO_3$







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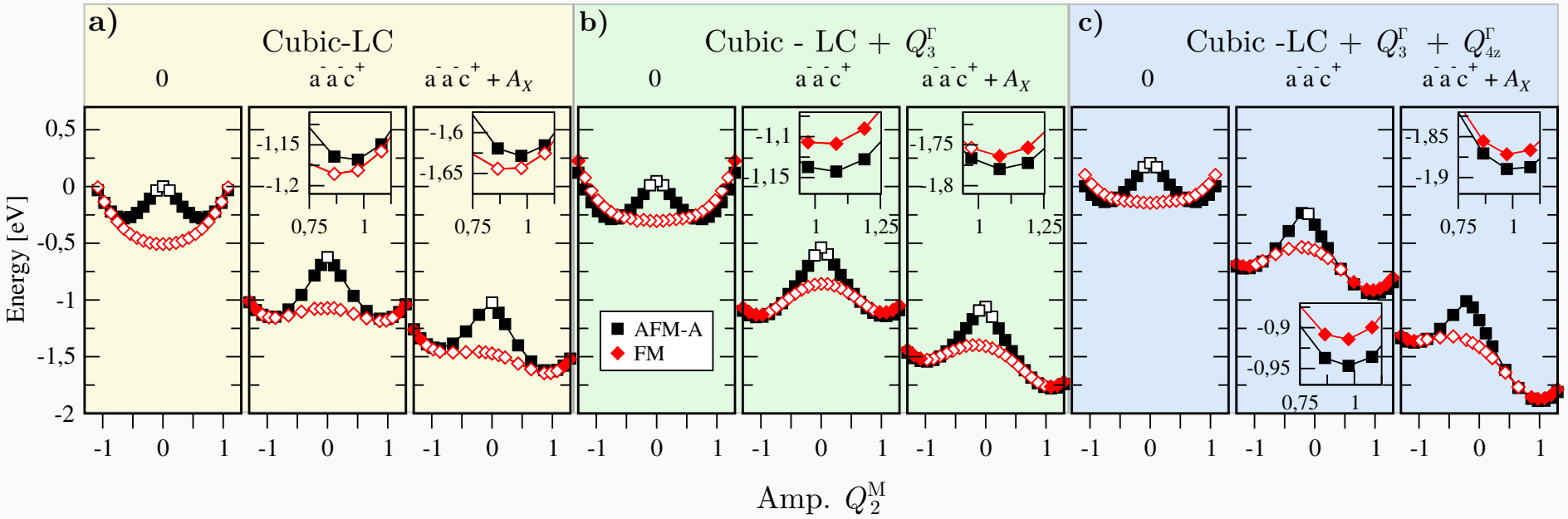
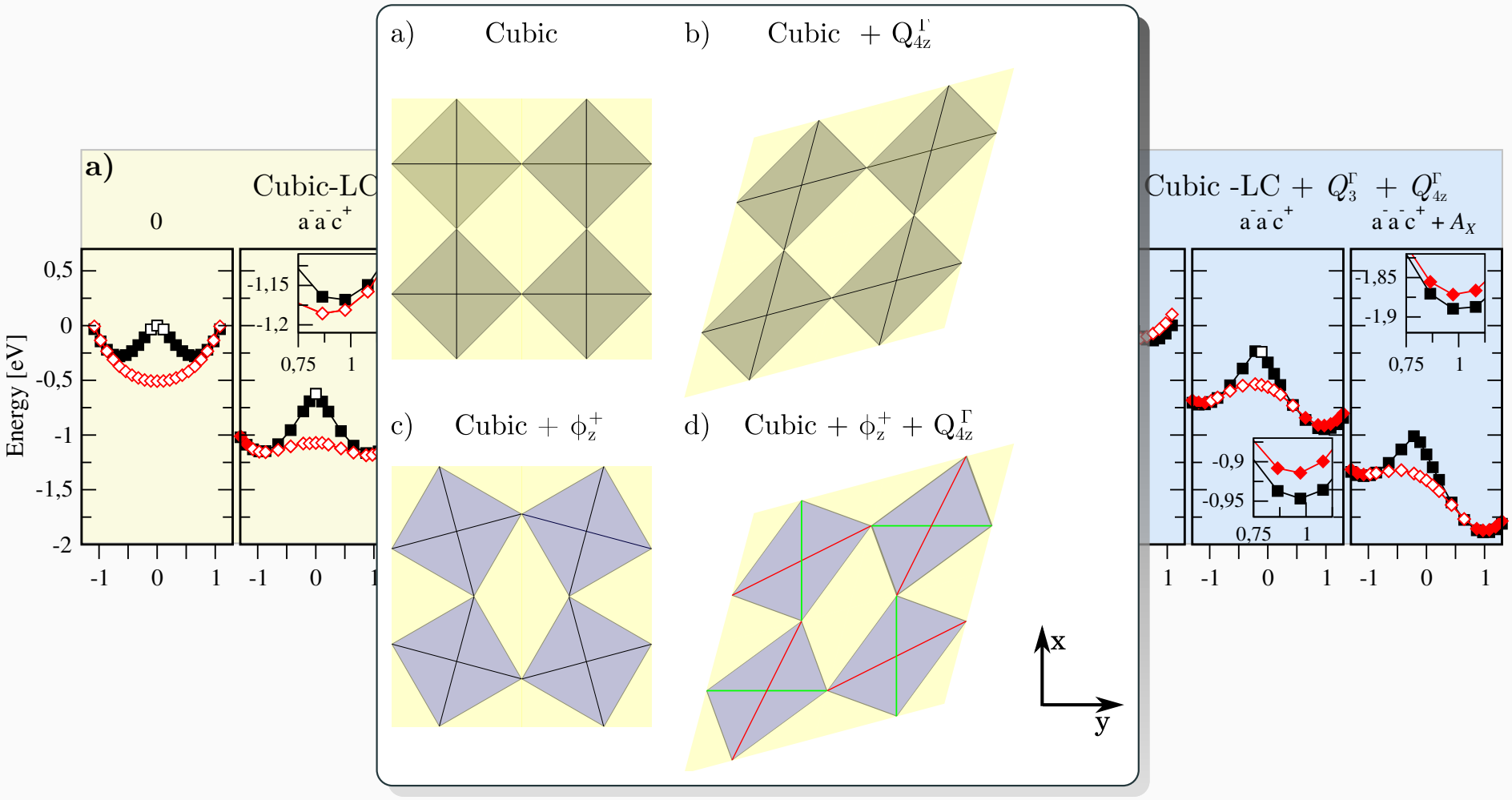
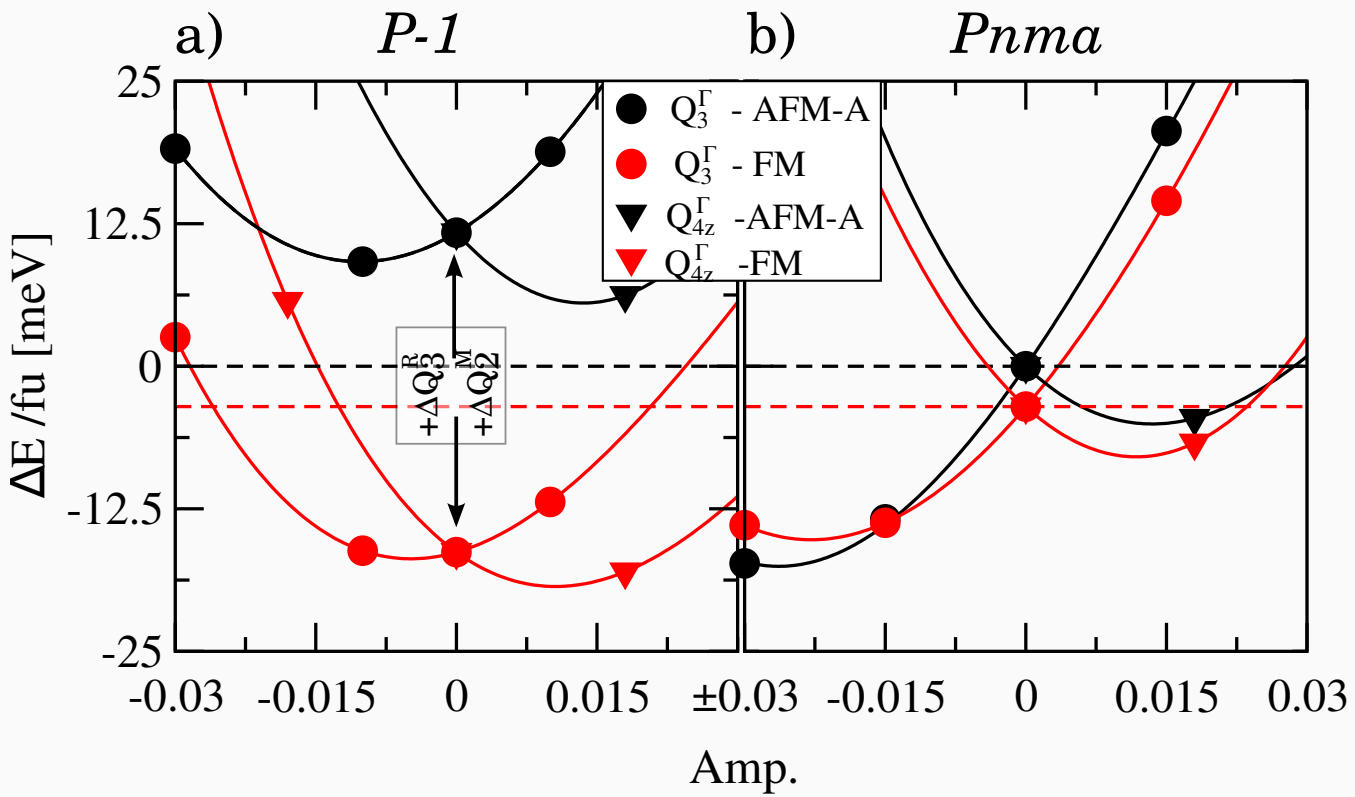
Full Potential Energy Surface $LaMnO_3$



Full Potential Energy Surface $LaMnO_3$

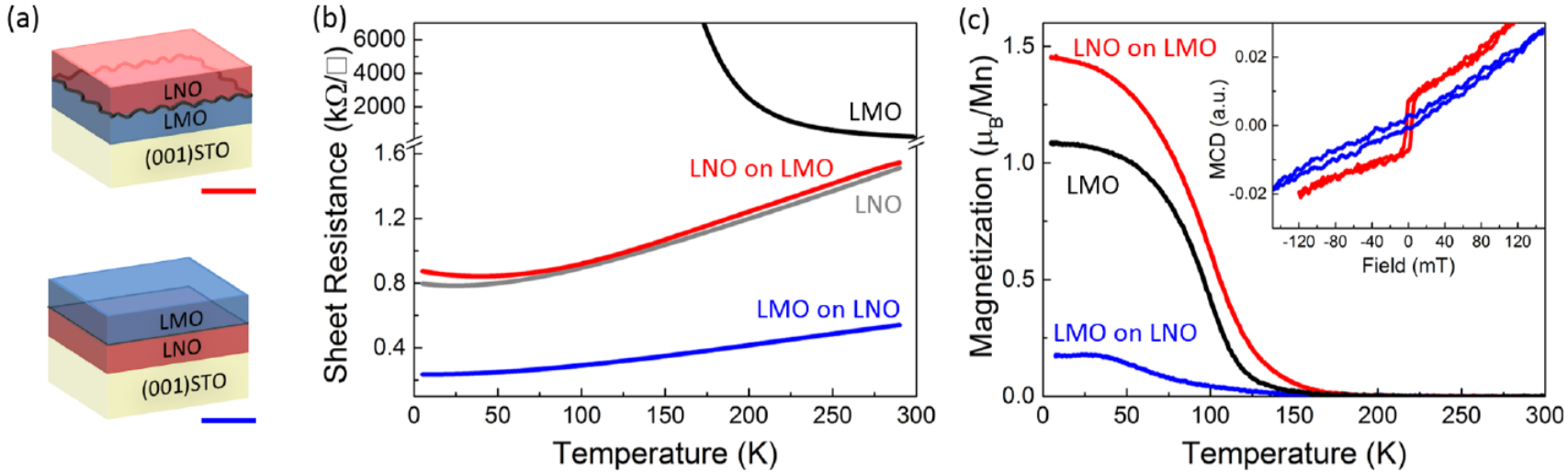


Strain PES



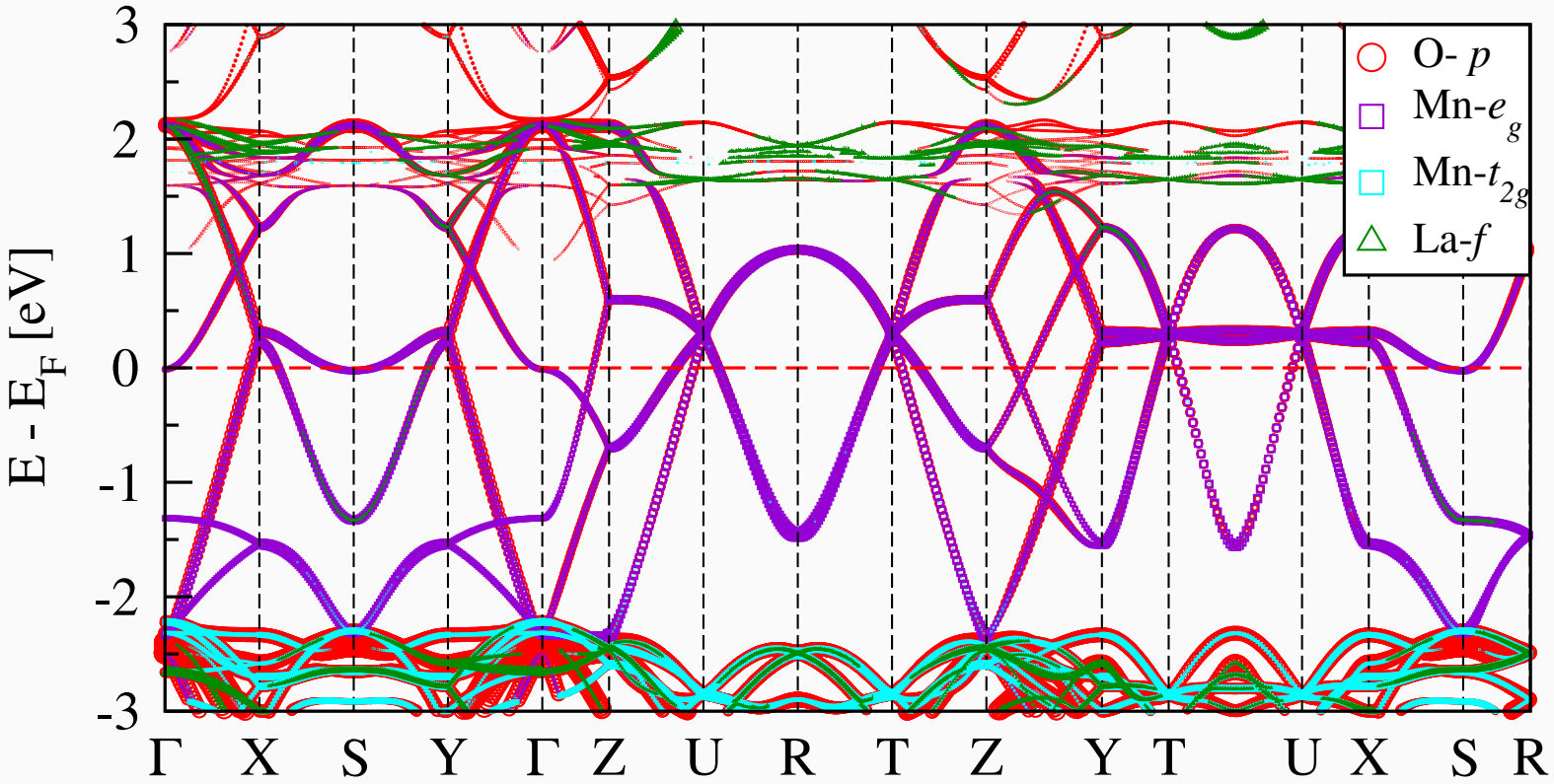
Phase	A_X[Å]	ϕ_z^+[Å]	ϕ_{xy}^-[Å]	Q_2^M[Å]	Q_3^Γ[Å]	E/fu[eV]
P-1	0.20	0.40	0.64	0.11	0.09	-31.744
Pnma	0.20	0.40	0.64	0.17	0	-31.728

$LaMnO_3$ $LaNiO_3$ Bilayers on $SrTiO_3$



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

Projected Band Structure



Influence of U|J Parameters