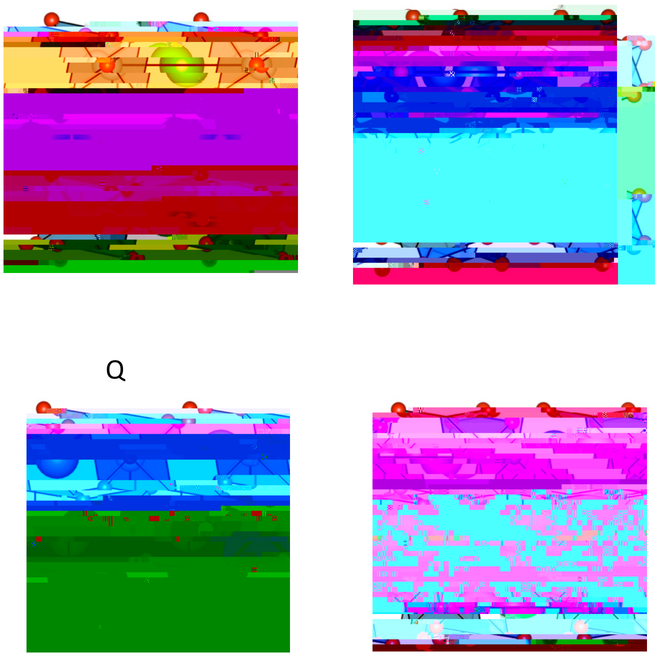
Origins versus fingerprints of the Jahn-Teller effect in *d*-electron ABX_3 perovskites

J [1,2] M B [1] A [3]


Q

(= O, F)

J -T $_2^-$ $_2^+$

. T

[7,10,21,34]

( )

O_3 [10]

3 [8,36]; ( )

$2\ O_3 \rightarrow\ _2$,

TABLE I. D ... - ... $_3$ ... E ... w GGA + HSE06 (OBS) w OBS ...). T ... OBS. AFM ... . R ... AFM ... , AFMG L T O_3, KF F_3, KC F_3; AFMC L O_3; AFMA L M O_3, KC F_3, KC F_3.

	E	($\sqrt{2}$, $\sqrt{2}$, 2) (GGA +)		P (HSE06)
		Δ OBS− OBS (/ . .)	( )	Δ OBS− OBS (/ . .)
L T O_3	^{1} ($\frac{1}{2}$ ↑)	0 (0)	0	0
L M O_3	^{4} ($\frac{3}{2}$ ↑ $\frac{1}{}$ ↑)	0 (0)	0	0
L O_3	^{2} ($\frac{2}{2}$ ↑)	−297 (−237)	0.42	−428
KF F_3	^{6} ($\frac{3}{2}$ ↑ $\frac{2}{}$ ↑ $\frac{1}{2}$ ↓)	−		

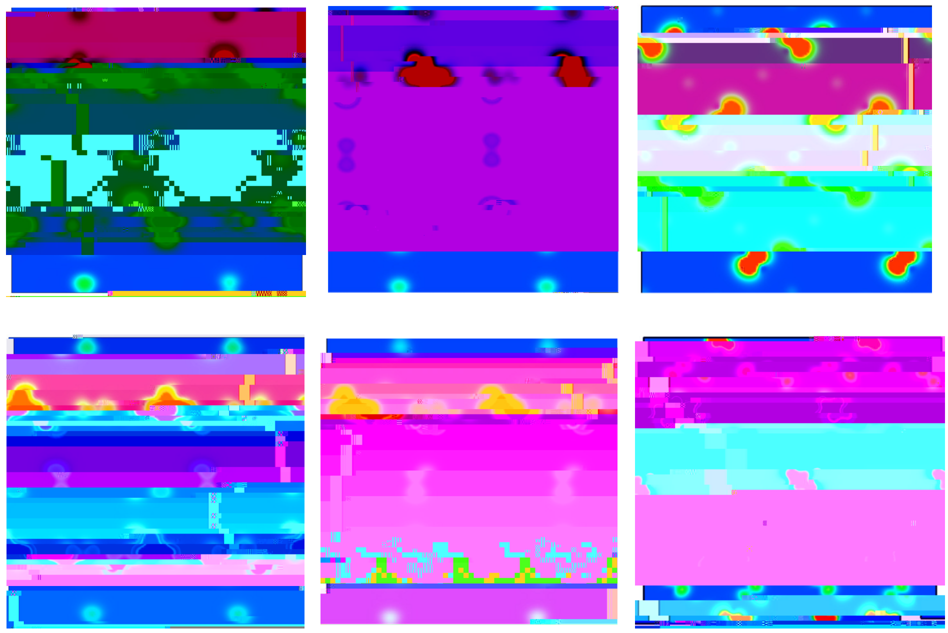


TABLE II. A [illegible] . T G [illegible] . E [illegible]

	Q	M Q	S Q	Q_2^+ (Q_3^+) C Q (E .)	Q_2^- (Q_3^-) C Q (E .)
L T O_3	0.93	AFMG	[illegible]	0.040 (0.041 56)	
L M O_3	0.94	AFMA	[illegible]	0.324 (0.357 30)	
L O_3	0.95	AFMC	2_1/	0.005 (0.009 57)	0.093 (0.079 57)
				0.078 (0.090 58)	
KF F_3	1.00	AFMG	2/		0.104 ( )
KC F_3	1.01	AFMG	1		0.003 ( )
KC F_3	0.99	AFMA	2/		0.336 (0.316 28)
			4/		0.300 (0.299 28)
KC F_3	1.03	AFMA	4/		0.335 (0.355 29)

C. The Q_2^+ motion in $LaTiO_3$ and $LaMnO_3$ is a consequence

F . 4(Q DMFT (F . 8 R . 3),

2. The origin of the improper Q_2^+ motion in LaMnO$_3$

O Q $^+_2$ Q Q Q . A , L M O$_3$ 3 Q Q C 30,64 . T Q Q ( ) Q Q L M O$_3$ J -T Q . O Q L M O$_3$ 750 K, R . 30 . U Q (A G Q). T Q Q–

*3. The origin of the orbital ordering in R*TiO$_3$ *(R* = Lu-La, *Y)*

A L M O$_3$, L T O$_3$ Q J -T Q. J R . 34 L T O$_3$ Q . T T- Q Q α + β , + γ α, β, γ Q Q Q (. .,) R . 34 .

D. Competing Jahn-Teller effect and sterically induced Q_2^+ mode is at the core of the entangled spin-orbital properties in RVO$_3$ compounds

A Q Q . T Q L O$_3$ Q T II), J -T O$_3$ (= L -L ,) Q . H , L O$_3$ Q . O Q O$_3$. C 21,55 , Q (Q + Q) O$_3$ 0 K. I Q , Q Q Q

Q J -T Q. C Q Q - AFM Q Q –S Q ($\sqrt{2}$, $\sqrt{2}$, 2) Q Q Q O$_3$ Q Q Q (S Q III A), -Q Q Q Q Q Q - AFM (Δ Q -Q = +31 / . .), Q - AFM (Δ Q -Q = −74 / . .). I Q 2 Q Q Q Q Q N . Q Q Q QQ (Q AFM), Q Q FM (Δ Q -Q = −34). T O$_3$ J -T Q . T 2$_1$/ Q Q Q T I R . 21 . T Q Q Q 0 K O$_3$? T ($\sqrt{2}$, $\sqrt{2}$, 2) Q QQ O$_3$

AFMG AFMC : ( ) $_2^+$

( ) $_2^-$

. T

$_2^+$ S III C

10

J -T (A H).

O

31,55

$_2^-$ $_2^+$

J -T

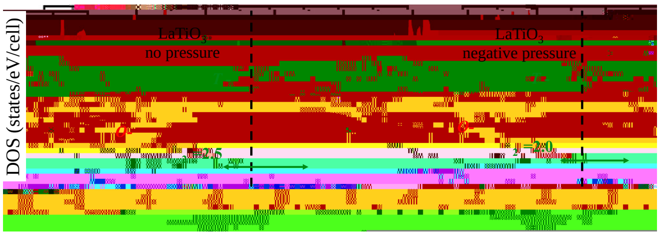


FIG. 6. P O T- L TO_3 ( ).

L TO_3). U , L TO_3 O T 2 (F . 6). F (Δ = −6 / . .).

APPENDIX C: ENERGY GAIN ASSOCIATED WITH Q_2^+ AND Q_2^- OCTAHEDRAL DEFORMATION MODE

S ($\sqrt{2}$, $\sqrt{2}$, 2) 3 4/) $\bar{2}$ $\bar{2}$

TABLE I . E ( ) . L . T FM .

	Δ_{2+} ( )	Δ_{2-} ( )
KF F_3	−2739	−2760
KC F_3	−2976	−3004
L O_3	−1153	−1325
KC F_3	−1295	−1298
KC F_3	−1019	−1020

3 4/) FM . E (20-) T I L O_3, KF F_3, KC F_3, KC F_3, KC F_3. T KC F_3 (AFMA 2 / . . KC F_3).

APPENDIX D: POTENTIAL ENERGY SURFACES ASSOCIATED WITH Q_2^-

F . 7 (0) FM .

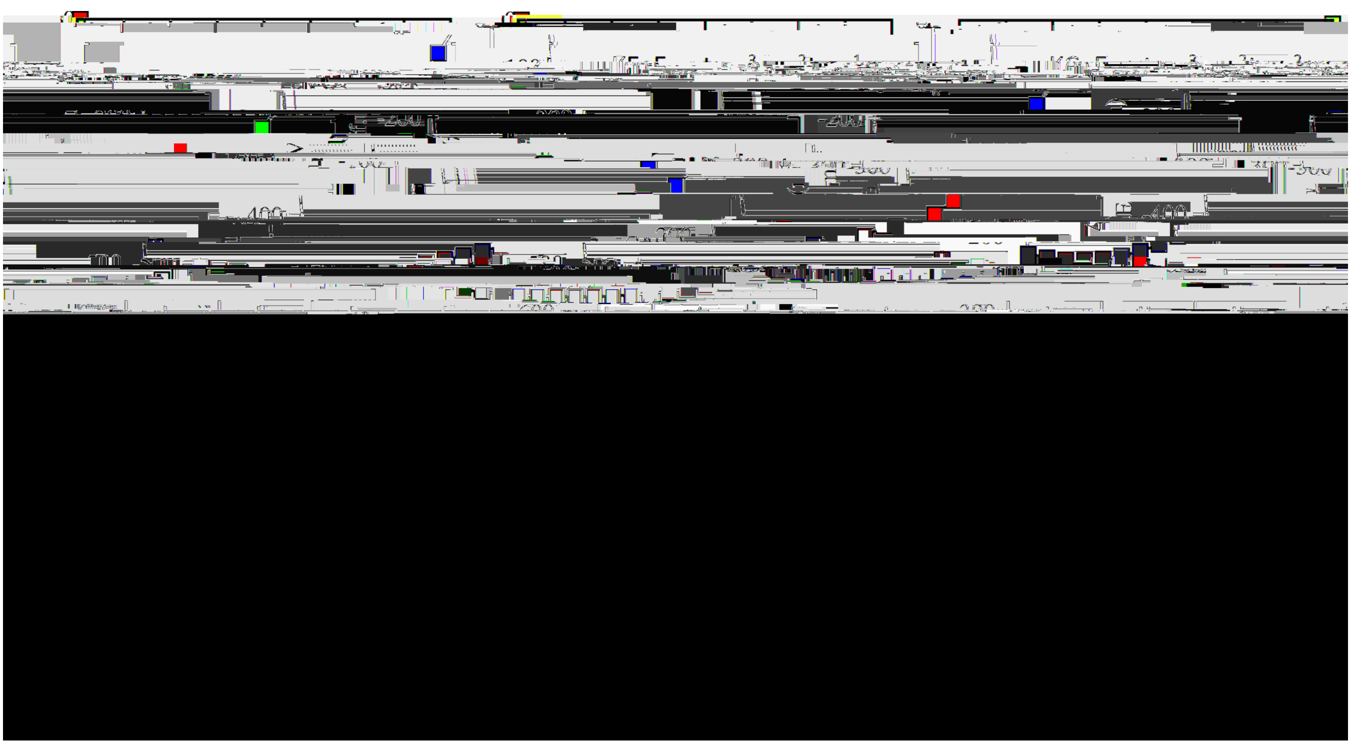


FIG. 7. P ($\sqrt{(2)}$, $\sqrt{(2)}$, 2) . P FM .

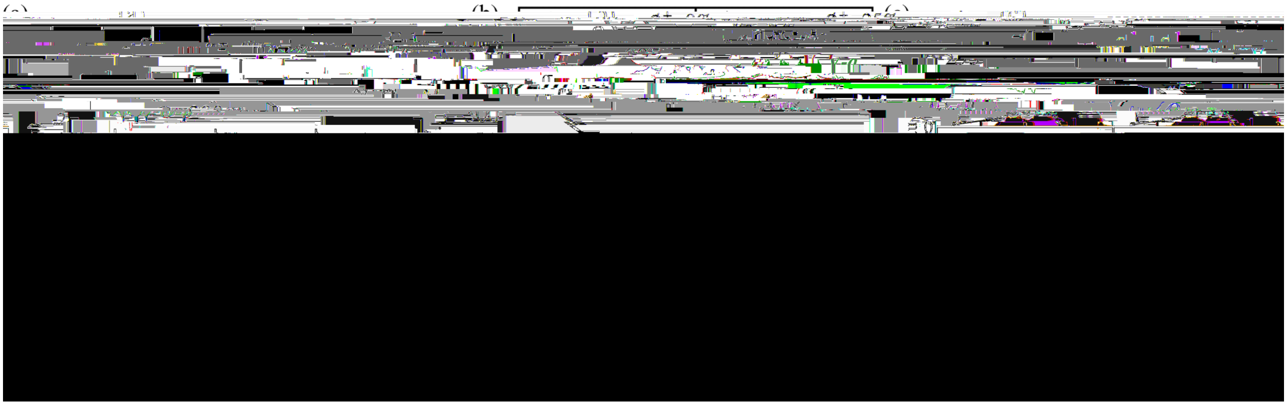


FIG. 9. C ... J -T ... L O_3. ( ) E ... L O_3 ... . H 0 ... . O ... . ( ) P ... ( ) / ( ), L O_3 ... . ( ) P ... ( ) O_4 ( ) ... . A FM ...

... (NM) ...). L ... (^{2}) ... (^{2}) ... . O ... (Δ = −9 / . .).

APPENDIX G: SYMMETRY MODE ANALYSIS OF $LaMnO_3$ EXPERIMENTAL STRUCTURES

... L M O_3 ... [30] ... ϕ^- ... ϕ^+ ... $^+_2$ ... . A ... R ... T ...

APPENDIX H: COOPERATING AND COMPETING OCTAHEDRAL ROTATIONS AND JAHN-TELLER EFFECT IN $LaVO_3$

I ... KC F_3 ... JTD (A E), ... L O_3. F ... JTD ...

... F . 9( ). T ... O_3 ... [31]: JT ... (. .,) ... . T ... : ( ) T ... ^{2} ... F . 9( ); 0 ... DFT ... ($\sqrt{2}$, $\sqrt{2}$, 2) ... ^{2} ... (,) I ... F . 9( ), ... (, ,) B ... , O ... JTE F . 9( ).

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