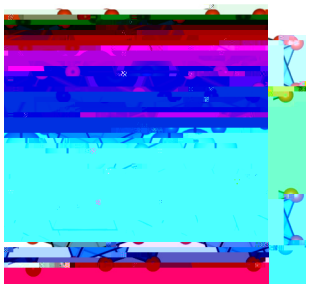
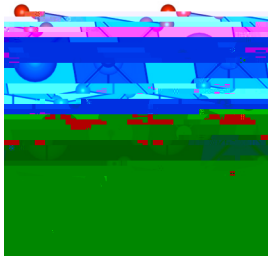
O e e f e Ja -Te e effec *d*-e ec *ABX*$_3$ e e

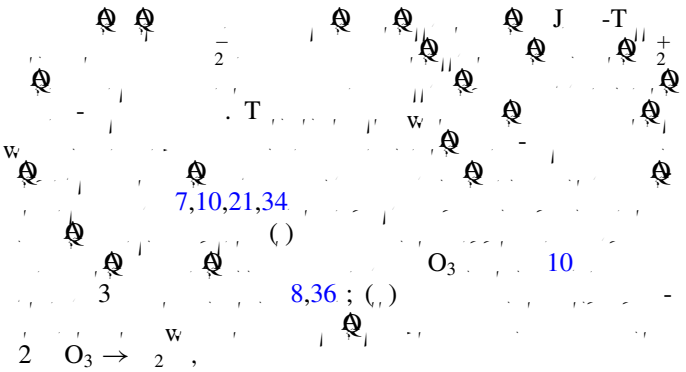
J ,[1,2] M B, [1] A [3]

[1]
[2]
[3]



Q





7,10,21,34

( )

O_3 10

3 8,36 ; (,) -

2 $O_3 \rightarrow$ 2 ,

TABLE I. D - . E w GGA + HSE06 (OBS) OBS OBS. A FM . 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.

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

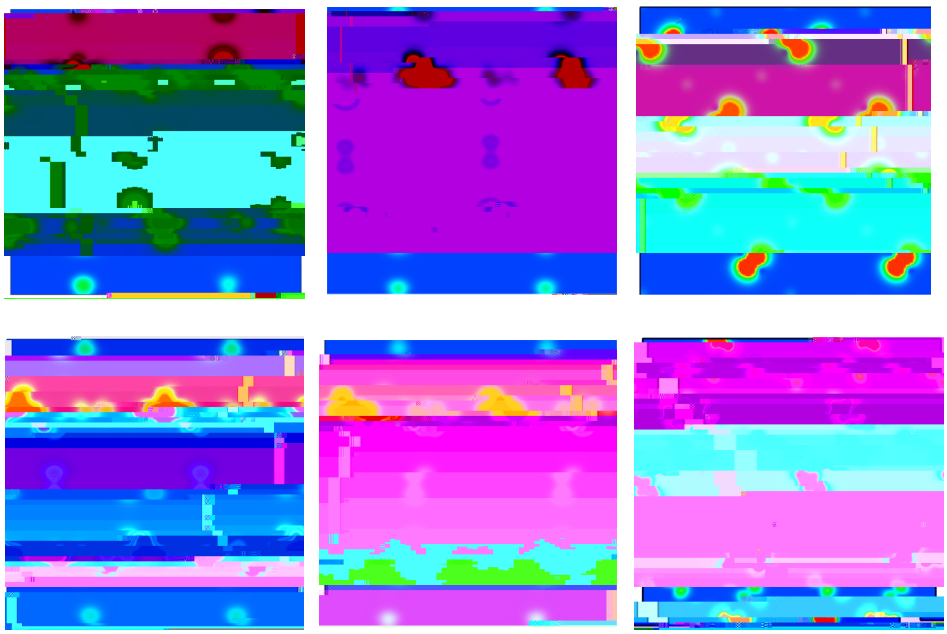


TABLE II. A ( ) . T G . E . A

		M	S	$\frac{+}{2}$ ($\frac{+}{3}$) C (E .)	$\frac{-}{2}$ ($\frac{-}{3}$) C (E .)
L T O_3	0.93	AFMG		0.040 (0.041 56)	
L M O_3	0.94	AFMA		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. T e Q_2^+ LaT O_3 a d LaM O_3 a c e e ce

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

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

O $\frac{+}{2}$
. A , L M O$_3$
3
ϕ^- C
30,64 . T
( ) J -T
L M O$_3$ ( ) 6
$\frac{+}{2}$
. O L M O$_3$
750 K,
R . 30
ϕ^- . U
(A G
). T
$\frac{+}{2}$

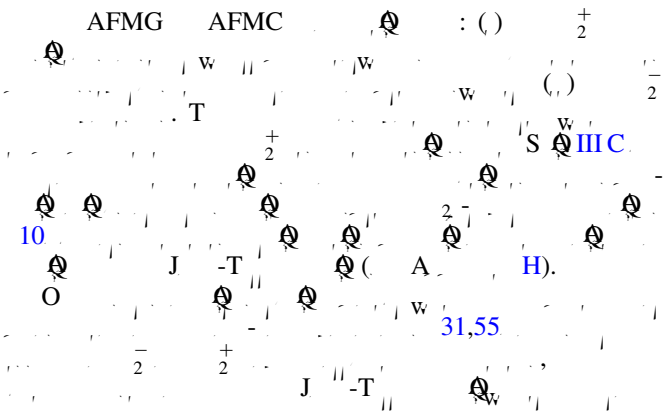
3. The origin of the orbital ordering in RT O$_3$ (R = L -La, Y)

A L M O$_3$, L T O$_3$
J -T . J
R . 34 L T O$_3$
$\frac{+}{2}$. T
T - α , $+\beta$, $+\gamma$
α, β, γ
(. .,)
R . 34 .

D. C e Ja -Te e effec a d e ca y d ced Q_2^+ de a e c e f ee a ed - b a e e RVO_3 c d

A $\frac{+}{2}$ $\frac{-}{2}$
, $\frac{+}{2}$
. T L O$_3$
(T II), J -T -
. H , O$_3$ (= L -L ,) -
, L O$_3$. O
6 O$_3$.
C 21,55 , (+) O$_3$
0 K.
I $\frac{+}{2}$, -

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



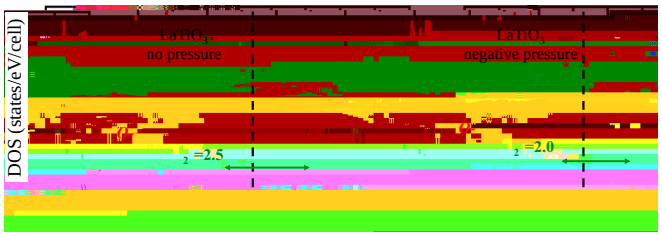


FIG. 6. P O ( ) T - ( ), L T O ( ) ( ).

L T O , (. .,). U , L T O O T 2 (F . 6). F , , KC F3 (Δ = −6 / . .).

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

S - ($\sqrt{2}$, $\sqrt{2}$, 2) $\frac{-}{2}$ $\frac{+}{2}$ 3 4/)

TABLE I . E ( ) $\frac{+}{2}$ $\frac{-}{2}$. 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

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

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

APPENDIX G: SYMMETRY MODE ANALYSIS OF LaM O$_3$ EXPERIMENTAL STRUCTURES

L M O_3 30 ϕ^- ϕ^+ $^+_2$. A R T .

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( ).

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

1. H. K , D. R. H. B (S , B , 2009).
2. D. I. K (C -T

8 G. T , Q , . , A. , P . R . B **97**, 035107 (2018).
9 G. M. D , , Q. L , J. , M. B , A. , P . R . B **98**, 075135