Origins versus fingerprints of the Jahn-Teller effect in *d***-electron** *ABX***³ perovskites**

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The Jahn-Teller distortion that c[an re](http://crossmark.crossref.org/dialog/?doi=10.1103/PhysRevResearch.1.033131&domain=pdf&date_stamp=2019-11-26)move electronic degeneracies in partially occupied states and results in

 $\mathsf Q$

Distinguishing features of the current approach. We address \mathbb{Q}^7 subject by subject by subject by subject \mathbb{Q}^7 and \mathbb{Q}^7 and \mathbb{Q}^7 materials (= O, F) with a transition-metal element exhibiting degenerate states (but with a properties to undergo the disproportionational disproportionational disproportionational disproportionation \mathbf{w}

TABLE I. Detection of a spontaneous electronic instability in the high-symmetry cubic phase of *ABX*³ perovskites. Energy differences between solutions with equal occupancy of \mathcal{R} and with the most state in meV per formula unit obtained obtai with GGA + and HSE06 \hat{Q} (the latter uses \hat{Q} , \hat{Q} $\hat{Q$ a relaxed cubic cubic cell with R are reported in particular are reported in particu L T_,O₃, KF₃, KC_{F3}; AFMC L O₃; AFMA LM_{O3}, KC_{F3}, KC_{F3}.

C. The Q_2^+ motion in LaTiO₃ and LaMnO₃ is a consequence

and the state of the state		

2. *The origin of the improper* Q_2^+ *motion in* LaMnO_3

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Ø. $\hat{\mathbf{\Theta}}$ ()	$\frac{1}{2}$ J. -T \int_{0}^{∞} L M O_3 $\pmb{\mathbb{Q}}^{ }$
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$\stackrel{+}{2}$	

3. The origin of the orbital ordering in RTiO₃ ($R = \text{Lu-La}$ *,* Y *)*

FIG. 6. Pro \bigcirc **q** equation of $O_{\mathbf{1}}$ levels (red area) and $O_{\mathbf{1}}$ T_{i} - levels (green area) in a cubic cell of \mathbf{Q} and \mathbf{Q} and \mathbf{Q} without \mathbf{Q} without \mathbf{Q} and \mathbf{Q} a $\frac{1}{\mathbf{w}}$ is a negative pressure (right panel).

 $\begin{array}{ccccc}\n & L T_1 O_{3w} & \cdots & v_{w-1} & \cdots & \cdots & \cdots & \cdots \\
& & \ddots & \ddots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
& & & 1 & 1 & 1 & 1 & 1\n\end{array}$ v_{w} is a volume expansion of \mathbf{v}_{w} , LaT_iO₃ st_{ill} $\frac{1}{\mathbf{w}}$ minimalistic hybridizations between $\frac{1}{\mathbf{w}}$ but the bandwidth associated with \mathbf{Q} levels is strongly is strongly is strongly is strongly in Θ_{w} respect to the unperturbed cubic cell (see Fig. 6). $F_{\mu_{\mathbf{Q}}^{W}}(x) = \mathbf{Q}$ tronic instability able to break orbital degeneracies able to break orbital degeneracies and to break orbital Θ produce a \mathbf{Q} -type antiferro-orbital arrangement is observed in the second is observed in the second is observed in the second of \mathbf{Q} $(\Delta = -6$ / f.

APPENDIX C: ENERGY GAIN ASSOCIATED WITH *Q***⁺ 2 AND** *Q***[−] ² OCTAHEDRAL DEFORMATION MODE**

L O_3 −1153 −1325 KC F₃ -1295 -1298 KC F₃ -1019 -1020

APPENDIX D: POTENTIAL ENERGY SURFACES ASSOCIATED WITH *Q***[−] 2**

FIG. 7. Potential energy surfaces as sociated with the condensation of a $\frac{1}{2}$ $\frac{1}{2}$ \mathbf{Q} or a product mode (arbitrary units) starting from a starti ($\overline{(2)}$, $\overline{(2)}$, are plotted using $\mathbb{F}M$ magnetic order.

FIG. 9. Coupling between rotations and Jahn-Teller effect in LaVO3. (a) Energy gain associated with breaking orbital degeneracies in Lo₃ as $\frac{\phi}{\phi}$ corresponds to the in-phase rotation of the in-phase rotation is added to the in-phase rotation is the material \mathbf{Q} (b) \mathbf{P} and \mathbf{Q} for different area) in LaVO₃ for different amplitudes of in-phase areas of in-phase areas of in-phase \mathbf{Q} for \mathbf{Q} for \mathbf{Q} for \mathbf{Q} for \mathbf{Q} for \mathbf octahedral rotations. (c) Projected density of states on V- levels (in red) and O-*p* levels (in green) for different amplitudes of an in-phase octahedral rotation. A FM order is used in all these simulations. The simulations of the simulations. The simulations of the simulations of the simulations of the simulations. The simulations of the simulations of the simu

APPENDIX G: SYMMETRY MODE ANALYSIS OF LaMnO3 EXPERIMENTAL STRUCTURES

APPENDIX H: COOPERATING AND COMPETING OCTAHEDRAL ROTATIONS AND JAHN-TELLER EFFECT IN LaVO3

tions since such since such since such situation preserves or \mathbb{Q}_p directions between consecutive planes along the propagations of \mathcal{Q} axis of the distortion. Our first-principles simulations \mathbf{Q} this hypothesis and starting from a cell with either a single $\mathbf{Q}_{\text{u},\mathbf{w},\mathbf{u},\mathbf{v},\mathbf$ in-phase or antiphase rotation, we observe a slightly larger a slightly larger a slightly larger a slightly la energy gain by breaking orbital degeneracies for the in-phase \mathbf{Q} and \mathbf{Q} in-phase \mathbf{Q} rotations that for the antiphase rotations (Δ = −9 meV/ \ldots between the two solutions). We nevertheless observe a surprising behavior with the \mathbf{W} prising behavior with the surprising behav

amplitude of the internal order of the electronic instability \mathbf{Q} , \mathbf{Q} , \mathbf{Q} , \mathbf{Q} , \mathbf{Q} breaking orbital degeneracies \mathfrak{g} increases upon i ing the rotation amplitude and then decreases for large rotation and then decreases for large rotation \mathcal{Q} amplitude \mathbf{F}_i g. $9($ and \mathbf{T}_i compatible compatible \mathbf{Q} is strictly compatible compa with the experimental phase O_3 Q compounds O_3 31 : $J \Gamma$ Q Q Q factor (i.e., the rotation amplitude) for \mathbf{Q} the strength of \mathbf{Q} $\begin{array}{ccc} \mathbf{\Theta} & \mathbf$ tation amplitude. This *a* priori unexpected behavior has the set of \mathbb{Q} origins: (i) The rotation amplitude first splits the degeneracy of \mathbf{Q} of the threefold-degenerate ²*^g* partners and the *xy* orbital is pushed to lower energies, leaving degenerate *xz*/ *yz* orbitals at higher energies $F_i = 9($ and $)$; note that at 0 rotation, the point group symmetry is already reduced from $\overrightarrow{DFT \bigoplus}$ $\overrightarrow{2}$, $\overline{2}$, 2) \overrightarrow{Q} , \overrightarrow{Q} $\mathbf{\mathfrak{Q}}_{\mathbf{u}\mathbf{W}}$ are alleady \mathbf{v} are already split 2 levels are already split \mathbf{v} are already split. \mathbf{Q} rotations reduces the bandwidth of the bandwidth of the degenerations reduces the degenerations of the degenerations \mathbf{Q} erate partners [Fig. 9(b)], and *de facto* the strength of the elec- $\mathbf{\mathbb{Q}}$ instance installer installer amplitude of \mathbf{B} and \mathbf{B} amplitude of rotations, \mathbf{O} p –V hybridization enters and decreases electron localization enters and decreases p JTE $F \cdot 9(\bigcirc$

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