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Orbital order in $La_{0.5}Sr_{1.5}MnO_4$: a failure of the local Jahn-Teller physics HUA WU, C.F. CHANG, O. SCHUMANN, Z. HU, Univ. Cologne, Germany, J.C. CEZAR, ESRF, Grenoble, France, T. BURNUS, N. HOLLMANN, Univ. Cologne, Germany, N.B. BROOKES, ESRF, Grenoble, France, A. TANAKA, Hiroshima Univ., Japan, M. BRADEN, D.I. KHOMSKII, Univ. Cologne, Germany, L.H. TJENG, MPI for Chem. Phys. Solids, Dresden, Germany — Orbital order (OO) occurs quite often in orbitally degenerate correlated transition-metal compounds. It has been generally accepted that there is one-to-one correspondence between a specific orbital order and a local Jahn-Teller distortion. Here we demonstrate that this is not always true, by demonstrating a failure of the local Jahn-Teller physics in the layered perovskite $La_{0.5}Sr_{1.5}MnO_4$ which is one of prototype OO materials. We studied both the site- and bond-centered charge orderings, crystal field levels, orbital states and their dependence on the varying local lattice distortions, through detailed *ab initio* electronic structure calculations. We conclude that this material has the site-centered charge ordering, and that the local Jahn-Teller physics fails and the type of occupied orbitals ($3x^2$-r^2/$3y^2$-r^2 ones) contradicts the local compression of $Mn^{3+}O_6$ octahedra which could require x^2-z^2/y^2-z^2 occupation. We explain this by the contribution of the long-range crystal-field in this anisotropic layered material and by the maximization of kinetic energy. Our theoretical results are confirmed by x-ray absorption linear dichroism.

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