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Electron interaction effects on Jahn-Teller instability in LaMnO₃¹ WEI-GUO YIN, Physics Department, Brookhaven National Laboratory, Upton, NY 11973, DMITRI VOLJA, WEI KU, Physics Department, Brookhaven National Laboratory, Upton, NY 11973 and Physics Department, State University of New York, Stony Brook, NY 11790 — We investigate the origin of the orbital ordering in LaMnO₃ using the LDA+U method and Wannier functions analysis. We find that electron-electron interaction dramatically facilitates the distortion of the MnO₆ octahedra and effectively enhances electron-phonon interaction. In addition, electron-electron interaction plays a significant role in determining real lattice distortion and orbital ordering pattern, beyond the conventional Jahn-Teller picture. Our conclusion agrees with existing experimental data and could be directly verified by future measurements, e.g., soft X-ray scattering.

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