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**Theoretical study of orbital and lattice structure of $MnF_3$: the origin of orbital ordering**[1] D. VOLJA, WEI-GUO YIN, WEI KU, Physics Department, Brookhaven National Laboratory, Upton, NY 11973 — Orbital ordering in $MnF_3$ is studied with first-principles theory. Mathematical description of $e_g$ states within pseudospin formalism shows the importance of electron-electron interactions that oppose conventional electron-phonon interactions (e.g.: Jahn-Teller effects). Results obtained with LDA+U give stable ground state with experimentally observed orbital ordering, that cannot be explained solely in terms of electron-phonon interactions. Instead, the resulting orbital ordering is a consequence of competition between electron-phonon and electron-electron interactions. Our quantitative conclusion can be directly verified in future experiments.

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