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Novel mechanism for displacive distortions in perovskites: On the orbital ordering transition in $KCuF_3$ HUNTER SIMS, German Research School for Simulation Sciences, EVA PAVARINI, Institute for Advanced Simulation, Forschungszentrum Jülich, ERIK KOCH, German Research School for Simulation Sciences — The Mott insulating perovskite $KCuF_3$ is considered the paradigmatic system with long-ranged orbital order and a cooperative Jahn-Teller distortion of the Cu-F octahedra. However, recent experiments have revealed that the JT-like distortions persist and even grow as temperature is increased. We show that neither superexchange nor Jahn-Teller can accurately describe this behavior—even qualitatively. Supported by GGA+U and model calculations, we explain this anomalous result in terms of a volume-driven lattice instability of purely ionic origin. We examine the effect of ionic size on this mechanism through the related systems $KCu_{1-x}Mg_xF_3$, $KCrF_3$, and $ACuF_3$. As a non-electronic effect, this instability should allow for octahedral distortions even in closed-shell systems with cubic ground states, and we propose design guidelines for the realization of this high-temperature broken-symmetry phase experimentally.

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