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The origin of hyper-ferroelectricity in LiBO_3 ($B=\text{V, Nb, Ta, Os}$)

LIXIN HE, PENGFEI LI, XINGUO REN, G-C GUO, University of Science and Technology of China — The electronic and structural properties of LiBO_3 ($B=\text{V, Nb, Ta, Os}$) are investigated via first-principles methods. We show that LiBO_3 are belong to the recently proposed hyperferroelectrics, i.e., they all have unstable longitudinal optical phonon modes. Especially, the ferroelectric-like instability in the metal LiOsO_3 is a limiting case of a hyperferroelectrics, whose optical dielectric constant goes to infinity. We further show via an effective Hamiltonian that in contrast to normal proper ferroelectricity, in which the ferroelectric instability usually comes from long range coulomb interactions, the hyperferroelectric instability is due to the structure instability driven by the short range interactions. This could happen in systems with large ion size mismatches, which therefore provides a useful guidance in searching for novel hyperferroelectrics.

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