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Strain induced structural, electronic, and magnetic properties of $SrFeO_2$ and $BaFeO_2$ WEIDONG LUO, XIAOLE ZHANG, Shanghai Jiao Tong University, China — The structural, electronic and magnetic properties of $SrFeO_2$ and $BaFeO_2$ under tensile strains are studied using first-principles density-functional theory calculations. Strain-induced Jahn-Teller-like behaviors involving the cooperative displacements of oxygen atoms are predicted in both compounds. Lattice dynamical properties are also investigated and the strain-induced imaginary phonon modes are consistent with the Jahn-Teller-like distortion. The usual Jahn-Teller instability of degenerate energy levels does not contribute to the interesting phenomena. Besides the structural and electronic properties, a transition of magnetic orderings from G-type anti-ferromagnetic phase to C-type anti-ferromagnetic phase is predicted in both compounds, which originates from the combined effects of the lattice-orbital coupling and the spin-orbital coupling due to exchange interaction between orthogonal Fe $3d$ orbitals.
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