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Poster : First-principles study of structural and vibrational properties of SrHfO₃ compared to SrZrO₃ (Computational Condensed Matter 20 (2019) e00383)

Abstract : The structural and vibrational properties of SrHfO₃ compared to those of the SrZrO₃ were investigated using first-principles calculations. The phonon dispersion curves, reported in the high-symmetry cubic perovskite phase, point out the coexistence of structural antiferrodistortive instabilities at the *R* and *M* zone-boundary points and a ferroelectric instability at the zone center. Different possible intermediate phases are characterized by comparing their internal energies, giving the same hierarchy of phases as for the SrZrO₃. The main features of the ferroelectric instability are also discussed, and, contrary to what was found for SrZrO₃, it seems very unlikely to induce the ferroelectricity in the SrHfO₃ *Pnma* ground state either by compressive or tensile epitaxial strain.