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The structure of $BaZrO_3$: a comparative first-principles study

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Summary

Using several popular first-principles packages for materials modeling the nature of the cubic lattice of barium zirconate has been investigated. The evaluated vibrational spectra typically exhibit an extended and prominent dynamical instability. The instability manifests through imaginary frequency optical modes along the whole R-M edge of the Brillouin zone. The experimentally observed simple cubic structure is found to be dynamically unstable against an antiferro-distortive transformation. The computations predict an orthorhombic crystal structure of the material, only slightly distorted from the cubic lattice, with an eight times larger unit cell and alternate ZrO_6 octahedra slightly rotated in opposite directions around the cartesian axes. The neglect of the barium $5s^2$ and $5p^6$ electrons in the valence configuration of Ba is found to be responsible for the previously reported incorrect results. Possible reasons for the observations of a stable cubic structure are discussed as well as the implications for the previously reported results. The ways to recover correct results from several previous studies that predicted the cubic structural model of BaZrO3 and to avoid potential pitfalls in the future are suggested.

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