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Effects of fluorine content on the elastic behavior of topaz [$Al_2SiO_4(F,OH)_2$]

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Abstract

In this work, we modeled the structure, the compressional behavior and the physical properties of topaz over six different fluorine contents and a wide range of pressure, using a quantum mechanical approach based on periodic boundary conditions. We adopted the density functional theory using the B3LYP functional and all-electron Gaussian-type orbitals basis sets. An atomic level description of the athermal (T = 0 K) pressure-induced structural modification of topaz is provided. From the compression results we obtained the athermal bulk modulus (K_{T0}), its first derivative (K') and the athermal volume at zero pressure (V_0) by a third-order Birch-Murnaghan equation fit. The results show that K_{T0} increases with fluorine content. The compressional pattern is anisotropic, as observed by the axial compressibility and second-order elastic constants calculations. We observed that the compression involves three different mechanism, polyhedral contraction, polyhedral tilting and hydrogen bonding, all of them influenced, with different extent, by the fluorine content in topaz. Recent experimental results obtained by single-crystal X-ray and neutron diffraction of specific topaz compositions are in very good agreement with our simulations, which further extend the knowledge of the structural and elastic properties of topaz over a wider range of fluorine content.

Keywords: Topaz, DFT, B3LYP, equation of state, elastic constants, athermal limit