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Effect of pressure on Zircon's ($ZrSiO_4$) Raman active modes: a first-principles study NATALYA SHEREMETYEVA, DANIELE CHERNIAK, BRUCE WATSON, VINCENT MEUNIER, Rensselaer Polytechnic Institute — Zircon is a mineral commonly found in the Earth crust. Its remarkable properties have given rise to considerable attention. This includes possible inclusion of radioactive elements in natural samples, which allows for geochronological investigations. Subsequently, Zircon was proposed as possible host material for radioactive waste management. Internal radiation damage in zircon leads to the destruction of its crystal structure (an effect known as metamictization) which is subject to ongoing research. Recently, the effect of pressure and temperature on synthetic zircon has been analyzed experimentally using Raman spectroscopy (Schmidt et al., Am. Min. 98, 643 (2013)) which led to the calibration of zircon as a pressure sensor in diamond-anvil cell experiments. While there have been a number of theoretical studies, the effect of pressure on the Raman active modes of zircon has not been investigated theoretically. Here we present a first-principles pressure calibration of the Raman active modes in Zircon employing density-functional theory (DFT). We find excellent quantitative agreement of the slopes $\partial\omega/\partial P$ with the experimental ones and are able to rationalize the ω vs. P behavior based on the details of the vibrational modes.

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