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A First Principles Approach to Modelling $\mathbf{Ba_{(1-x)}Ca_{(x)}ZrO_3}$ JOSEPH BENNETT, ILYA GRINBERG, ANDREW RAPPE, University of Pennsylvania — Dielectric properties are often optimized by varying material composition, so there is a need to understand the impact of doping on the local structure and properties of a material. One study showed that the dielectric constant of $BaZrO_3$ (BZ) can be increased by up to 50% by doping with small amount of Ca [1]. This is interesting because $CaZrO_3$ (CZ) actually has a lower epsilon than BZ. We use first principles methods to characterize the local structure of $Ba_{(1-x)}Ca_{(x)}ZrO_3$ (BCZ) at various compositions and compute the contribution to the dielectric response of each normalized mode at 0 K. There arise low frequency phonon modes related to Ca-O motions and a transformation of Raman modes to IR modes caused by the introduction of Ca. [1]Levin, I. et al. J Sol. State Chem. 175 (2003) 170-181

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