A First Principles Approach to Modelling $\text{Ba}_{(1-x)}\text{Ca}_x\text{ZrO}_3$

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 $\text{BaZrO}_3$ (BZ) can be increased by up to 50% by doping with small amount of Ca [1]. This is interesting because $\text{CaZrO}_3$ (CZ) actually has a lower epsilon than BZ. We use first principles methods to characterize the local structure of $\text{Ba}_{(1-x)}\text{Ca}_x\text{ZrO}_3$ (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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