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A Density Functional Theory Calculation Of The Oxygen Vibration Mode Frequencies In CdTe[1] WEI CHENG, Univ. of Calfiornia-Berkeley, LEI LIU, Nanyang Technical University, PETER YU, Univ. of California-Berkeley, Z.X. MA, Lawrence Berkeley National Lab, SAM MAO, Univ. of California & LBNL
— The vibrational frequencies of oxygen impurity in CdTe have been calculated for a variety of oxygen environments using first-principle density functional theory. The local mode of an isolated oxygen atom substituting for Te is found to have a frequency of 331.86 cm^{-1} as compared with the experimental value of 349.8 cm^{-1}. Two high frequency modes (at around 1104 cm^{-1}) have previously been identified with the vibrational modes of a complex consisting of a substitutional oxygen and a neighboring Cd vacancy. We found that the frequencies of such oxygen-complexes are far too low to explain the experimental results. In stead we found that the frequency of an oxygen molecule or dimmer located inside a Cd vacancy is in good agreement with experiment.

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