Identifying the High Frequency Local Modes in Oxygen Doped CdTe & CdSe with *ab initio* Density-Functional Theory

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Abstract

Oxygen is a common contaminant in CdTe thin film solar cells. Since oxygen atoms are much lighter than the Te atoms they replace, the vibration modes of oxygen in the CdTe lattice are highly localized around the oxygen atoms and have been labeled local modes. A group at Purdue University has reported unusually high frequency local modes in CdTe (>1000 cm^{-1}) and CdSe (>2000 cm^{-1}) samples doped with oxygen. [1,2] The identification of these high frequency modes has remained controversial.[3]

We have performed first principle DFT calculation to study the vibrational mode and formation energy of oxygen in CdTe and CdSe. We found that the vibration of oxygen molecules can explain the >1000 cm^{-1} modes in CdTe and CdSe. For the >2000 cm^{-1} modes in CdSe they can be explained by the vibration of OH radicals located inside Cd vacancies. The existence of these high frequency modes suggests possible contamination of the CdSe samples by water vapor during growth.

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