

IR spectroscopy of O-related defects in CdSe

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Detailed infrared (IR) absorption spectroscopy of O₂-related defects in zincblend-CdTe and wurtzite-CdSe were reported by Lavrov *et al* [Phys. Rev. B **84**, 233201 (2011), AIP conf. Proc. **1583**, 169 (2014)]. They clearly showed based on their experimental work that the IR absorption bands at 1096.8 and 1108.4 cm⁻¹ in CdTe samples are associated with the vibrational modes of SO₂-related defects in CdTe. In wurtzite-CdSe, due to the reduction in the symmetry (in comparison to the zincblende structure), there are three absorption peaks at 1094.2, 1107.5, and 1126.3 cm⁻¹ related to the SO₂ defects, instead of two. T-Thienprasert *et al* [J. Appl. Phys. **115**, 203511 (2014)] recently showed that SO₂ in CdTe can form a complex defect with Cd vacancy becoming SO₂-V_{Cd} complex defects with the vibrational frequencies in good agreement with the values observed by Lavrov *et al*. In this work, we employed first-principles calculations to study the SO₂-related defects in wurtzite-CdSe. Their formation energies were calculated and used to analyze the stable ones. The vibrational frequency associated with each defect were calculated via the frozen-phonon approximation and used to compare with the observed values. In wurtzite-CdSe, We found that the SO₂ defects can bind with V_{Cd} becoming SO₂-V_{Cd} complex defects similar to the case of SO₂ in CdTe. However, due to the lower symmetry of wurtzite structure, there are many possible orientations of SO₂-V_{Cd} complex defects, which will be presented along with their formation energies as well as calculated vibrational frequencies.

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