The effect of oxygen impurity on the electronic and optical properties of calcium, strontium and barium chalcogenide compounds

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Abstract
Electronic and optical properties of calcium, strontium and barium chalcogenide compounds in NaCl structure are studied using the band structure results obtained through the full potential linearized augmented plane wave method. Different linear relationships are observed between theoretical band gap and 1/a² (where a is lattice constant) for calcium, strontium and barium chalcogenide compounds with and without oxygen, respectively. An abnormal behavior of electronic and optical properties are found for compounds containing oxygen. These effects are ascribed to the special properties of Ca-O, Sr-O and Ba-O bonds, which are different from chemical bonds between Ca, Sr and Ba and other chalcogen atoms.

Keywords: DFT, FP-LAPW, Chalcogenides, optical properties, electronic properties, band gap

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