First principles calculations for vacancies and antisites in PbSe and PbTe: bulk and nanowire

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The energetic stability and the electronic properties of vacancies (V_X) and antisites (X_Y) in PbSe and PbTe are investigated. PbSe and PbTe are narrow band gap semiconductors and have the potential to be used in infrared detectors, laser, and diodes. They are also of special interest for thermoelectric devices (TE). The calculations are based in the Density Functional Theory (DFT) and the General Gradient Approximation (GGA) for the exchange-correlation term, as implemented in the VASP code. The core and valence electrons are described by the Projected Augmented Wave (PAW) and the Plane Wave (PW) methods, respectively. The defects are studied in the bulk and nanowire (NW) system. Our results show that intrinsec defects (vacancies and antisites) in PbTe have lower formation energies in the NW as compared to the bulk and present a trend in migrate to the surface of the NW. For the PbSe we obtain similar results when compare the formation energy for the bulk and NW. However, the Pb vacancy and the antisites are more stable in the core of the NW. The intrinsec defects are shallow defects for the bulk system. For both PbSe and PbTe V_{Pb} is a shallow acceptor defect and V_{Se} and V_{Te} are shallow donor defects for the PbSe and PbTe, respectively. Similar electronic properties are observed for the antisites. For the Pb in the anion site we obtain an *n*-type semiconductor for both PbSe and PbTe, Se_{Pb} is a *p*-type for the PbSe, and Te_{Pb} is a *n*-type for PbTe. Due the quantum confinement effects present in the NW (the band gap open), these defects have different electronic properties for the NW as compared to the bulk. Now these defects give rise to electronic levels in the band gap of the PbTe NW and the V_{Te} present a metallic character. For the PbSe NW a *p*-type and a *n*-type semiconductor is obtained for the V_{Pb} and Pb_{Se}, respectively. On the other hand, deep electronic levels are present in the band gap for the V_{Se} and Se_{Pb}. These results show that due an enhanced in the electronic density of states (DOS) near the Fermi energy, the defective PbSe and PbTe are candidates for efficient TE devices.