Contribution ID: **31** Type: **Poster**

Optical features of semiconducting crystal Hg3S2Br2: first-principles investigation

Saturday, 26 September 2020 14:18 (4 minutes)

First-principles calculations based on the density functional theory (DFT) were carried out to investigate the electronic and optical properties of semiconducting crystal Hg3S2Br2. The electron exchange-correlation energy was described by the generalized gradient approximation (GGA) and modified Becke-Johnson (MBJ) potential. The analysis of the band energy dispersion shows that the optical band gap is estimated to be roundly 2.69 eV. It is in satisfactory agreement with experimental value of 2.9 eV. The band topology near the conduction band minimum is changed due to the spin-orbit coupling in the mercury orbitals at the Γ-point of the Brillouin zone. The essential contribution into the energy of the Hg-S bond adds the hybridization of sulfur p orbitals that are oriented along the bond. However, some contribution to the bond between the [SHg3] trigonal pyramids of the [Hg3S2Br4] octahedra also came from hybridization of p orbitals of sulfur atoms that form neighbor pyramids. Using the calculated dispersion of the real and the imaginary parts of the complex dielectric function, one can determine other optical properties such as absorption coefficient α(ω), refractive index n(ω), extinction coefficient k(ω), energy loss function L(ω) and reflectivity R(ω). The first crucial point of the optical absorption edge emerges in the visible light (at about 5 eV) and, with enhancing photon energies, the region with high absorption expands up to the 33 eV revealing the formation of some spectral features emerging due to different optical transitions.

Topics

Session A. Physics of condensed matter and spectroscopy

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Session Classification: Poster session