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Trends in Evolution of the Energy Band Structure of Chalcopyrite $CuB^{III}X^{VI}_2$ Compounds with Variation of the B and X Compositions

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Abstract

Bulk and nanostructured $A^IB^{III}X^{VI}_2$ chalcopyrite materials, including quantum dots on their basis, are widely used in the development of optical filters, solar cells, optoelectronic devices and photocatalysis. Physical properties of both bulk and nanostructured chalcopyrite compounds are determined by their energy band structure. The optical spectroscopy is one of the powerful and nondestructive method for determination of physical properties. This paper presents results of investigation of optical reflectance spectra of $CuB^{III}X^{VI}_2$ compounds with B = Al, Ga, and In, and X = S and Se, performed in a wide spectral range from 1.7 eV to 7.5 eV. The measured spectral position of peaks in the reflectance spectra are assigned to electronic transitions in different points of the Brillouin zone, on the basis of the electronic band structures of these materials deduced from theoretical calculation performed in previous works. Trends in the evolution of the energy band structure with changing the composition of materials have been revealed, which are important for practical applications. Apart from that, the observed trends in the evolution of the energy band structure of chalcopyrite $CuB^{III}X^{VI}_2$ compounds with variation of their composition are helpful for a right assignment of the observed peaks in the reflectance spectra to respective electronic transitions in various points of the Brillouin zone.

Keywords: chalcopyrite materials, solid solutions, optical reflectance spectra, energy band structures, brillouin zone, electronic transitions

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