Calculation of electronic structure of vacancies and their replacements in semiconductors A3B6.

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Obtaining radiation-resistant materials with good electric and optical characteristics is an actual problem of modern physics. It is connected with development of nuclear power, flights in space, ecology and etc. Materials in these conditions under the strongest influence of various radiations change their physical properties, therefore radiation defects are formed. Restoration of properties of such materials demands studying of nature, properties of defects, and reasons of their formations. In this work the electron structure of defect semiconductors A3B6 is theoretically investigated. It have been calculated the electronic structure of local defects-vacancies and their replacement by the Green's function method on the basis of Bond Orbital and Linear Combination of Atomic Orbital (LKAO). Energy levels in the forbidden gap, in the band of conductivity and in the valence band were defined. Change of electronic density in semiconductors GaS, GaSe, InSe in the presence of anion and cation vacancies and replacement of these vacancies were calculated. Results of both methods are well agreed. The presence of anion and cation vacancies in these semiconductors leads to deep energy levels in the forbidden gap and also to levels in a valence band and in a band of conductivity. The calculated bound states in the forbidden gap with respect to the valence band top are: 0.2 eV, 0.4 eV, 0.6eV for Ga vacancy and 0.1 eV, 0.5 eV for S vacancy in GaS , 0.6 eV, 0.8 eV for Ga vacancy and 0.4 eV, 0.5 eV for Se vacancy in GaSe, 0.2 eV, 0.5 eV, 0.6 eV for In vacancy and 0.3 eV, 0.4 eV for Se vacancy in InSe. From the change of density's graphics resonances and antiresonances within the valence band for semiconductors A3B6 are defined. It have defined, that at replacement of vacancy by atom of an element of the same subgroup which ionic radius less than ionic radius of the replaced atom, for example, at replacement of atom Tl on cation vacancy in semiconductors GaSe and GaS, the local levels formed from vacancies completely disappear. Using this mechanism it is possible not only to restore former parametres of a crystal and to improve its characteristics. The received results are well agreed with experimental data.

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