Ab initio calculations for electronic structure engineering of Bi diluted III-V compounds and $Ge_{1-x}Sn_x$ alloy

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Modern optoelectronics is stimulated to a large extent by the development of optical fiber telecommunication. E.g. transmitters or receivers are devices based on semiconductor nanostructures. Semiconductor alloys are materials of promising perspective in the field due the possibility of controlling technologically their structural and electronic properties. The knowledge of material properties is crucial at the stage of device design. Large scale *ab initio* calculations based on Density Functional Theory (DFT) offer an opportunity of predicting the properties. The main limitation of the research tool is the size of the system under investigation. However, valuable and helpful scientific information can be obtained from calculations for cell-periodic bulk, where, owing to translational symmetry, the system can be represented by a limited number of atoms. The presentation will focus on chosen aspects of *ab initio* modeling of the structural and electronic properties, on the example of III-V-Bi diluted systems and $Ge_{1-x}Sn_x$ alloy [1-5]. In particular such characteristics like composition dependent lattice parameters, band structures, band offsets, have been calculated and suitability of the systems for optoelectronic applications predicted. Moreover, in the case of $Ge_{1-x}Sn_x$ alloy the electronic properties have been studied in the full range of compositions, the effect of ion distribution discussed and a contribution of various physical processes to the band-gap bowing evaluated.

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