Intervalley hybridization and optical properties of $Ge_{1-x}Sn_x$ quantum dots

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The $Ge_{1-x}Sn_x$ alloy attract much attention due to its band gap dependence on the composition. At some critical Sn content (of a few percent), the bulk changes its character from the indirect- to the direct band gap [1, 2]. The other properties of $Ge_{1-x}Sn_x$, like high carrier mobility, makes this material interesting from the point of view of applications for optoelectronic devices [3].

We present a theoretical, atomistic study of electron and optical properties of $Ge_{1-x}Sn_x$ nanostructures. Within the $sp^3d^5s^*$ tight-binding model, we calculate the electron and hole states in $Ge_{1-x}Sn_x$ cubic boxes and colloidal quantum dots. We investigate the interplay of confinement effect and composition-induced indirect-direct band gap transition. We demonstrate an intervalley hybridization of the ground electron state and identify the relevant regimes of sizes and QDs compositions, where they are optically active. We also calculate the absorbance spectra of experimentally-relevant colloidal quantum dots [4].

The simulations are performed within the $sp^3d^5s^*$ tight-binding model [5] combined with the valence force field model to account for strain in the system. We find the parameters via fitting the target Ge, α-Sn and zincblende GeSn band structures calculated using DFT approach with MBJLDA functional [2].

References

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