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Accurate model of Si-Ge-Sn alloys:Electronic and Optical properties

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Abstract content
   (Max 300 words)

A method based on the tight-binding linear muffin-tin orbital (TB-LMTO) and the Quasiparticle Self-consistent GW (QSGW) approximation is discussed. The goal is to obtain accurate electronic and optical properties of semiconductor alloys.
In this new approach, the parameters of the TB-LMTO Hamiltonian are used to fit the difference in the QSGW self-energies and the LDA exchange-correlation potentials. As such, the method possesses the accuracy of the QSGW approximation and the efficiency of the TB-LMTO.
We use the new Hamiltonian to interpret the optical transitions in Si-Ge-Sn alloys.

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