Simulation of optical excitation spectra of semiconductor nanowires within effective bond orbital model

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Abstract

Systematic studies of optical excitation spectra of semiconductor nanowires (including group IV, III-V, and II-VI materials) obtained by using an eight-band effective bond-orbital model (EBOM) are presented. A new set of EBOM parameters are determined which produce good band structures of zincblende semiconductors for the entire Brillouin zone, suitable for modeling the excitation spectra from infrared to ultraviolet. The band structures and optical excitation spectra, including both the interband and intraband transitions (for doped cases) are calculated. The calculations were done with the use of a symmetrized basis functions which transform according to the irreducible representations of the underlying point group. This can improve the computation efficiency by about two orders of magnitude. Thus, the electronic and optical properties of a large class of materials can be simulated.

Keywords

Author Keywords: Effective bond-orbital model; Nanowire; Optical absorption; Solar cell

KeyWords Plus: QUANTUM-WELLS; INFRARED PHOTODETECTORS; ELECTRONIC-STRUCTURE; BAND-STRUCTURE; SUPERLATTICES; WIRES; DOTS; ZNSE; ZNTE

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