A computational study of electronic and excitonic properties of quasi-one-dimensional superlattices. Seel, M.; Liegener, C. M.; Foerner, W.; Ladik, J

Abstract

Periodic copolymers representing quasi-one-dimensional superlattices (AmBn)x were studied within the tight-binding approxn. The LCAO approach was used to calc. the splitting into subbands, the widths of the subbands, and the no. of subbands in the well as a function of segment lengths m and n (barrier and well width). The Stark shift of subbands and the perturbed Wannier functions for a (A16B32)x superlattice were calcd. for various elec. field strengths using perturbation theory. Exciton resonances and the shift in exciton excitation energies due to an applied elec. field were computed by using a PPP parameter for the electron-hole interaction. The parameters for the empirical tight-binding calcns. were detd. from fully self-consistent Hartree-Fock calcns. and first-principles Green's function calcns. for the exciton energies for superlattices of shorter segment lengths. For the Stark shift of the exciton peak a red shift of .apprx.25 meV for 2×10^5 V/cm was calcd., similar to the shifts calcd. and obsd. in 3-dimensional superlattices.