SOLAR QUEST

SEMINAR ANNOUNCEMENT

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SYMMETRY REDUCTION IN MULTIBAND HAMILTONIANS FOR SEMICONDUCTOR QUANTUM DOTS: THE ROLE OF INTERFACES AND HIGHER ENERGY BANDS

DATE: Thursday, May 9, 2013
TIME: 10:00 am-12:00 pm
PLACE: Seminar Room A-502
CCR Building, 5F

ABSTRACT

In contrast to a popular belief that multiband envelope function **k·p** Hamiltonians cannot capture the right symmetry of zinc blend QDs, we show the opposite. The symmetry group of 8-band **k·p** Hamiltonian applied to a pyramidal square-based QD is the C4v group. We show that the inclusion of interface band mixing effects leads to the reduction of symmetry from an artificial C4v, to the correct C2v one. Our analytical derivations, demonstrate that interface effects lead to the reduction of symmetry from C4v to C2v since commutation [D(Rφ),H(if)]=0, only if φ = $n\cdot\pi$, where D is the group representation generators. The main manifestation of interface effects are the energy level splitting between (e1, e2), (h0, h1), and (h4, h5) states of the order of 1-3 ~meV in InAs/GaAs material system. The splitting decrease as the dot size and consequently the volume to surface ratio increase. The inclusion of the additional bands beyond the standard 8 bands also leads to symmetry reduction to C2v, with splitting which are however weaker than the ones due to interfaces. We have found analytically that the 14 band **k·p** Hamiltonian commutes with the operators of the C2v group representation, i.e. [D(Rφ),H(14 **k·p**)]=0 only for φ=$n\cdot\pi$. We have found indeed that the 14-band **k·p** Hamiltonian is the lowest order multiband Hamiltonian whose kinetic part has the correct C2v atomistic symmetry. This symmetry reduction originates from the coupling between the top of the valence (Γ5v) and the second conduction (Γ5c) band. The observed splittings are comparable to the ones that originate from spin-orbit coupling (these do not reduce the symmetry) and are much smaller than the ones from piezoelectric effect in strained systems. From the many body Hamiltonian constructed from configuration interactions (CI) using single electron orbitals with correct C2v symmetry, we have quantified that the fine structure splitting (FSS) between two bright excitons in the triplet is 6.4 micro eV due to interface effects and 4.7 micro eV due to explicate inclusion of the second conduction band of the underlying constituent materials (InAs and GaAs). Our work provides a very important conceptual message – with appropriate treatment of relevant effects, the multiband envelope function Hamiltonians are fully capable of capturing the right atomistic symmetry of QD structures.

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