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Efficient Modeling of Excitons in Type-II Nanowire Quantum Dots

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In nanowires, crystal phase quantum dots (QDs) can be synthesized by modifying the crystallographic structure as is shown in figure 1 [1]. This structuring can be made with atomic monolayer precision, and this good control of the geometry makes QDs in nanowires attractive systems for engineering quantum dot-based functionalities such as quantum gates. The crystallographic interfaces usually feature Type II band alignment, where electrons and holes are spatially separated onto the different polytypes, which is a key asset in implementing quantum gates. However, it also leads to very small oscillator strength (OS) in these structures compared to Type-I QDs.

In this work, we calculate exciton binding energy and oscillator strength using a full configuration interaction (CI) description of the few particle electron-hole system. Whereas widely used methods such as ab initio or tight binding are numerically demanding, the CI method is more efficient and thus suitable for engineering and design of quantum devices. We show that by engineering of a nanowire in double well QDs (DWQD) configuration, the oscillator strength, which is a key parameter in optical quantum gating in the STIRAP (stimulated Raman adiabatic passage) process for implementing quantum gates [2], is increased up to 10 times compare to single well QDs (SWQD). The initial ingredients of CI method for calculating the exciton state are the electron and hole single-particle wavefunctions and energies, which are obtained from the solutions of the three-dimensional Schrodinger equation within the envelope-function and effective-mass approximations. The few-particle Hamiltonian is then expanded within the bases of single-particle states. The exciton state is obtained by direct diagonalization of this Hamiltonian.

Figure 2 shows a nanowire DWQD bandstructure in the growth direction (z) and its schematic in the inset. Figure 3 shows the calculated exciton wavefunction in the electron and hole coordinates in the z direction which shows the exciton is bounded in the barrier between quantum dots in the z_h coordinate. By changing the interdots distance, the normalized OS of the bound exciton can be increased up to 50%, as is shown in Figure 4, which is 10 times larger than what is calculated for ground state exciton in SWQDs.

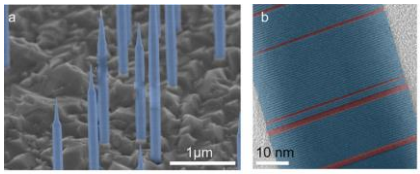

Fig. 1 Scanning electron microscope image of the grown crystal phase InP nanowire QD.

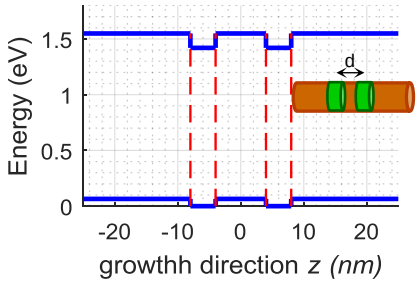

Fig. 2 InP nanowire DWQD band structure and its shematic in inset. Band structure parameters are from [1].

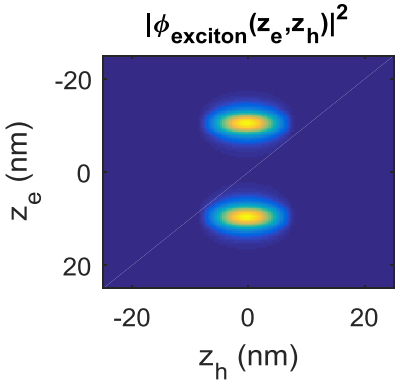

Fig. 3 Bound exciton state in the z coordinate of electron and hole.

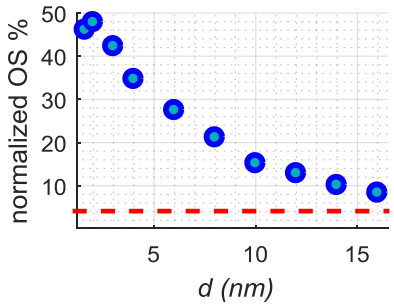

Fig. 4 Normalize OS vs interdot distance d in nanowire DWQD. Dash red line shows normalized OS in nanowire SWQD.

References

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