# II-VI SEMICONDUCTOR QUANTUM DOT QUANTUM WELLS: A TIGHT-BINDING STUDY

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We have developed a symmetry-based tight-binding (TB) method for calculating the electronic structure, exciton states and optical spectra in spherical semiconductor quantum dots (QD's).
It is based on the semi-empirical sp^{3}s^{*} model, including thespin-orbit interaction. The TB parameters of the QD Hamiltonian are those used to reproduce the bulk semiconductor band structure. The surface dangling bonds are passivated by hydrogen-like atoms in a controlled manner. We write the TB Hamiltonian in a block-diagonal form by using group-theoretical techniques. Exact diagonalization then yields the full single-particle spectrum including the symmetry classification of the eigenstates. We next introduce the (many-body) electron-hole interaction: both the Coulomb (direct) and exchange terms are considered. The low-energy exciton spectrum is then deduced in the configuration-interaction approach by diagonalizing the full exciton Hamiltonian in the single electron-hole pair excitation subspace of progressively increasing size until numerical convergence of the lowest excitonic energies. The electric dipole transition probabilities are also calculated. We thus obtain the low-energy fine structure characterizing the resonant and non-resonant photoluminescence Stokes shifts.

The method has so far been applied to CdSe [1] and CdTe [2] NC's of diameter up to 6 nm. Our theoretical results show a good agreement with the available experimental data on the size dependence of the fundamental gap and the Stokes shift, and provide a unified picture of the optical properties of small-size spherical QD's.

This good agreement between theory and experiment in binary NC's encouraged us to investigate more complex systems such as quantum dot quantum wells (QDQW's) for which no satisfactory atomistic theory was previously reported. We have studied three classes of QDQW's. One of them, CdS/HgS/CdS, is based on a CdS core which acts as a barrier, with a thin HgS well layer intercalated between the core and a clad layer of CdS. In addition to the characteristic spatial localization of carriers, our results for these CdS/HgS/CdS NC's show that, if we keep the total number of atoms fixed, the gap decreases when the well radius decreases [3]. The second class of QDQW's is based in ZnS cores. Several ZnS/CdS and ZnS/CdS/ZnS samples have been investigated in Ref. [4]. In these compounds, when a small ZnS core is covered with one or two CdS monolayers, the analysis of the density of states (DOS) and the wavefunctions near the gap edges reveals a strong influence of the CdS well. The ZnS/CdS/ZnS present a similar behavior: Even with only one CdS layer the DOS

projected onto the CdS region is large and the hole is mostly trapped in the well, but the electron is less trapped. With two CdS layers the DOS in the well is bigger than in the core and clad together for states near the gap edges which govern the physics of the systems. The calculated values of the absorption onset show a good agreement with the experimental data. Large photoluminescence Stokes shifts are also predicted [5]. Finally, very recent experimental results [6] incited us to undertake the study of the third class: CdS/CdSe/CdS QDQW's. The experiments reveal the spin dynamics and quantum size levels using time-resolved Faraday rotation (TRFR). Our preliminary results about the excitonic transitions are consistent with the resonance energies in the TRFR experimental spectra [7].

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