Atomistic modeling of multimillion atom nanosystems

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Fully ab-initio modeling of multimillion atom nanostructures such as quantum dots in nanowires [1] is still beyond the reach of modern computers. Yet, we show that accurate, atomistic modeling of electronic and optical properties of such systems is possible with the use of empirical tight-binding method for the calculation of single particle states combined with the valence force field simulation of strain fields and the configuration interaction method aiming for description of many-body effects [2,3]. The use of modern massively-parallel computers enables us to calculate excitonic complexes spectra of InAs/GaAs and InAs/InP quantum dots built-into quasi-one-dimensional nanowires, including the details of exciton fine structure [4], understanding of which is a necessary step towards efficient quantum dot based schemes of entangled photon pairs generation [4]. Our approach gives us a predictive capability for determining or tailoring nanosystems that poses demanded electronic or optical properties before actual experiment is performed.

References

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