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Atomistic Pseudopotential Calculations of the Electronic and Optical Properties of Self-Assembled Quantum Dots[1]

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The optical spectrum and the charging energies of semiconductor quantum dots have been recently measured with high accuracy. Both of these experimental techniques probe many-body states that are not directly described by independent particle theories such as the density functional theory. On the other hand, quasi- particle theories that can in principle address the problem, such as GW, are computationally too demanding for the study of nanostructures (as opposed to clusters) where many thousands of atoms are involved. One way to approach this problem is to use the effective mass approximation or the k.p method and choose a confinement potential that reproduces a few known experimental facts (e.g. the splitting between confined levels). These methods can provide a good initial guess but were shown to be too crude to enable a quantitative comparision with recent experiments. We therefore adopt a bottom-up atomistic approach where instead of starting from a simplified approach, such as effective mass, and progressively increase the complexity by adding parameters, we start from the accurate atomistic description (LDA or GW) and work ourselves up using a few well controlled approximations.
I will first present the method, namely (i) the scheme that is used to derive the empirical pseudopotentials including the piezoelectric effect, (ii) the choices that have to be made for the basis used to expand the wave functions, (iii) the inclusion of corelations through Bethe-Salpeter-like treatment. I will then present recent applications of the theory to calculate the fine-structure [1] of excitons and charged excitons, the charging spectra of holes [2] and the degree or entanglement stored in a quantum dot molecule [3].

[1] G. Bester, S.V. Nair, A. Zunger, prb **67**, 161306 (2003).
[2] L. He, G. Bester, A. Zunger, PRL (in press).
[3] G. Bester, J. Shumway, A. Zunger, PRL **93**, 047401 (2004)

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