

DIELECTRIC EFFECTS ON TWO-ELECTRON ENERGETIC STRUCTURE OF COLLOIDAL NANOCRYSTALLITES

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Colloidal synthesis of quantum dots yields spherically-shaped nanocrystallites with characteristic sizes down to 2 nm of diameter. A large amount of charge can be induced at the boundaries of these small nanostructures if the surrounding medium has a small dielectric constant [1]. Since the pioneer works by Brus and Stern [1,2], many experimental [3,4] and theoretical [5-7] efforts have been carried out in order to understand the role of these dielectric effects and to incorporate them as a designing tool in nanotechnology.

In this work, we calculate the energetic structure of two electrons confined in homogeneous and inhomogeneous (antidot) spherical nanocrystallites. In our calculations, self-energy and polarization effects induced by the dielectric mismatch at the heterojunctions are included. We carry out a CI calculation of bielectronic states. The one-particle basis set is provided by an exact (numerical) EMA calculation. We use a realistic (finite step-like) 3D spatial confining potential and position dependent electron effective mass. We find that the dielectric nature of the external medium strongly influences the energy ordering and spatial distribution of specific excited states. These effects depend on the topology of the heterostructure (quantum dot or antidot). The obtained results may be of interest for new applications based on the tailoring of the nanocrystallite properties by means of the design of the external dielectric medium.

References:

- [1] L.E. Brus, J. Chem. Phys. **80** (1984) 4403.
- [2] F. Stern, Phys. Rev. B **17** (1978) 5009.
- [3] G. Goldoni, F. Rosi, and E. Molinari, Phys. Rev. Lett. **80** (1998) 4995.
- [4] A. Orlandi, M. Rontani, G. Goldoni, F. Manghi, and E. Molinari, Phys. Rev. B **63** (2001) 045310.
- [5] P.G. Bolcatto, C.R. Proetto, J. Phys.: Condens. Matter. **13** (2001) 319.
- [6] G. Allan, C. Deleure, M. Lannoo, and E. Martin, Phys. Rev. B **52** (1995) 11982.
- [7] J.L. Movilla and J. Planelles, Phys. Rev. B **71** (2005) 075319.