Report finale

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Descrizione dettagliata dell'Istituzione ospitante: Centro Ricerca S3 (c/o Dipartimento di Fisica dell'Università di Modena e Reggio Emilia, via Campi 213/A - Modena), Istituto Nanoscienze del Dipartimento Materiali e Dispositivi, Consiglio Nazionale delle Ricerche

Periodo: 3 ottobre 2010 – 13 ottobre 2010

Titolo del programma:

Modellizzazione del rilassamento di stati multieccitonici in nanocristalli cilindrici: dagli effetti di correlazione alle proprietà di fotoconversione. (Modeling of multiexcitonic states relaxation in nanorods: from correlation effects to light-harvesting proprieties)

Relazione dell'attività scientifica svolta (in inglese):

In this project we have developed, test and run computational tools to simulate the optoelectronic properties of exciton complexes confined in cylindrical nanocrystal embedded in complex dielectric environments. In particular, we have focused on hybrid nanostructures formed by semiconductor quantum dots attached to metalic bodies.

Hybrid metal-semiconductor nanostructures have been successfully synthesized in the last years. The interest of these systems arises from the fact that one can take advantadge of the properties of the different materials or properties which are unique to the hybrid system and are not present for the separate components.[1-3]

Several applications have been envisaged for these structures. In particular, hybrid quantum dot-metal nanostructures have proved to be promising for photocatalytic activity.[4]

At present, understanding of the electronic properties of metal-semiconductor quantum dots is mostly restricted to experimental studies.[5] From the theoretical point of view, modeling these structures is a challenge. The behavior of carriers confined in the semiconductor depends on the 3D geometry of the quantum dot. By contrast, the carriers trapped in the metal redistribute over its 2D surface. Any theoretical model dealing with these systems should then be able to offer simultaneous and reliable description of volumetric states, surface states, and the electrostatic interaction between them.

Following the visit of Prof. Bertoni to the Quantum Chemistry Group of Universitat Jaume I (Spain, September 2010), the two groups have joined efforts to develop a pioneering computational tool to simulate optical excitons confined in such a system. The semiconductor carriers (electrons and holes) are modeled with an effective mass model. The electron-hole

Coulomb interaction is taken into account using Configuration Interaction codes developed in the CNR-Nano group. Finally, the electrostatic potential arising from the inhomogeneous dielectric environment, as well as from possible charges trapped in the metal, are calculated by integrating the generalized 3D Poisson equation. To this end, we are using the numerical method presented in Ref.[6].

The numerical integration of both Schroedinger and Poisson equations relies on a finite differences scheme. The grid employed in the integration must be fine enough to properly describe density charges near the metal surface. This poses the problem of solving huge and dense systems of linear equations of rank ~300,000. To solve this formidable problem, we have developed a code which relies on secondary memory storage. The linear system is solved using LU factorization with PLAPACK and its out-of-core extension, POOCLAPACK.[7]

We have built these libraries in the Cineca Supercomputing Center, where we have succeeded in solving systems of the desired rank with moderate virtual memory requirements.

By ensembling the efficient linear system solver with the suit of codes for studying hybrid nanostructures, we have been able to test the numerical accuracy of the physical results that can be reached with our tool. In the next stage, after the guest researcher stay in Modena, we plan to run simulations of excitonic states in nanorods with a gold cap or core-shell nanorods and compare with the results of partner experimental groups.

[1] K. Okamoto et al. Nature Mater. 3, 601 (2004).
[2] X. Qiu et al. J. Am. Chem. Soc. 129, 11908 (2007).
[3] T. Mokari et al. Science 304, 1787 (2004).
[4] R. Costi et al. Nano Lett. 8, 637 (2008).
[5] D. Steiner et al. Phys. Rev. Lett. 95, 056805 (2005).
[6] J.L. Movilla et al. Comp. Phys. Comm. 181, 92 (2010).
[7] J.M. Badia et al. submitted to Comp. Phys. Comm.

Firma del Proponente .....