

**21. СИМПОЗИЈУМ ФИЗИКЕ  
КОНДЕНЗОВАНЕ МАТЕРИЈЕ**  
**THE 21st SYMPOSIUM ON  
CONDENSED MATTER PHYSICS**

**BOOK OF ABSTRACTS**



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# 21. СИМПОЗИЈУМ ФИЗИКЕ КОНДЕНЗОВАНЕ МАТЕРИЈЕ

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## THE 21st SYMPOSIUM ON CONDENSED MATTER PHYSICS



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# Effect of Large Quantum Correlations in “Russian Doll” Quantum Dots: Impact on MEG Solar Cells

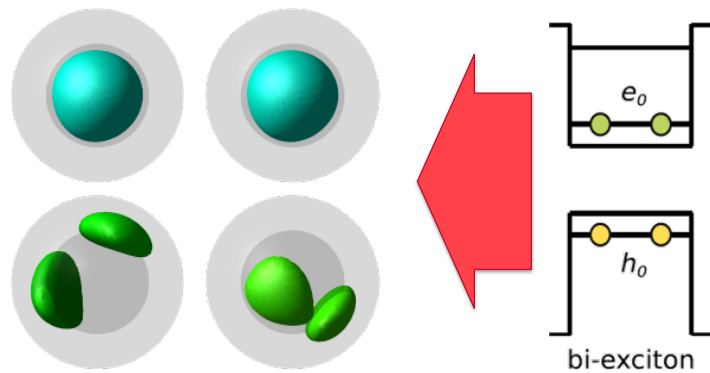
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**Abstract.** Semiconductor nanocrystals (NCs) are the subject of intensive research due to several novel properties which make them of interest for both fundamental science and technological applications. NCs are of particular interest for solar cell applications due to their ability to increase efficiency via the generation of multiexcitons from a single photon. Theoretical predictions indicate that multi-exiton generation (MEG) has the potential to enhance the efficiency of a single gap cell from 33% to 42% [1]. The efficiency of MEG in colloidal QDs is determined by the competition between MEG and other hot electron-cooling processes [2]. These have characteristic times of  $\tau(\text{MEG}) \sim \tau(\text{cooling}) \sim 1$  ps in the colloidal QDs studied to date but for the high efficiency  $\tau(\text{cool}) \gg \tau(\text{MEG})$  is required. The “Russian Doll” aka core/shell QDs [3] with type II band alignment offers extra degree of freedom in mediating both the optical dipoles and the Coulomb interaction between charges in such structures. Full realization of this potential requires that the energy threshold for MEG be minimized. An attractive interaction between excitons in QD reduces the threshold by the biexciton binding energy,  $B_{xx}$ , but this has been found to be small ( $-10$  meV) for type I QDs. Here, we show that, by taking into account quantum correlation effects between charges, combinations of core diameter and shell thickness can be found for a CdSe/CdTe core/shell QD that result in very large values of  $B_{xx} < 0$ . In our analysis excitonic states were found using the full Configuration interaction (CI) method, that includes explicitly the effects of Coulomb interaction, exact exchange and correlations between many-electron configurations in QD. In setting up the full CI, particular attention was paid to accurate modeling of the dielectric environment variation through the structure as well as surface polarization effects on core/shell and QD/colloid interfaces. Dielectric constants of constituent CdSe and CdTe around the transition energies poles are predicted using ab initio TDDFT [4]. We map the  $1S^{(e)nS^{(h)}}$  ( $n = 1, 2$ ) exciton correlation energy relative to the strong confinement regime as a function of core radius and shell thickness for non-uniform spatial dielectric environment [5]. We observe how the type-II confinement potentials amplifies the dielectric effect on the wave functions and exciton energies, particularly increasing the correlation energy for QDs in which the corresponding single-particle hole is delocalized [5]. We also find that correlation leads to large changes in the momentum matrix element, particularly for the lowest CdSe/CdTe QD exciton in which it is increased up to one order of magnitude in the presence of dielectric confinement. Overall dielectric confinement affected the exciton properties in CdSe/CdTe QDs more than the inverse heterostructures due to the band alignment, which encourages holes to localize in the shell. We conclude that: (i) it is not possible to predict biexciton binding using the Hartree approximation alone; it can only be predicted with a full CI Hamiltonian [6]; (ii) CI predicts  $B_{xx} = -70$  meV for structures with 0.5 nm thick shell that agrees with experiment [7]; (iii) by ignoring the dielectric confinement, it is not possible to predict biexciton binding for structures with shell thickness  $> 0.75$  nm; (iv) by changing the solvent’s dielectric constant from 1 to 2 the variation in the  $B_{xx}$  binding energy is as

big as 100 meV; (v) a proper prediction of Bxx requires the inclusion of correlations and surface polarization effects but the effect of self-polarization is negligible. The strong biexciton binding found in Russian Doll QD is explained by the stronger reduction in the Coulombic repulsion between holes than reduction in the attraction between electrons and holes upon the addition of the CdTe shell layer, Fig. 1. The Aufbau principle and Hund rule reveal this to be a consequence of 4 fold degeneracy of the hole ground state imposed by symmetry of the structure [8].

The peak efficiency in “Russian Doll” NC structures grows to 46% and then to 47% as Bxx increases to  $-25$  and  $-50$  meV, respectively. The largest biexciton interaction energy reported to date is  $\sim 100$  meV, although this was repulsive (i.e., antibinding) rather than attractive, it gives an indication of the magnitude of the biexciton interaction energies that can be achieved in “Russian Doll” type-II colloidal QD. For a binding energy of  $-100$  meV, the peak efficiency rises to 50% and would rise to as much as 60% if it was possible to produce a binding of  $-200$  meV. It can also be observed that the value of  $E_g$  corresponding to the peak efficiency shifts progressively to lower values as the photocurrent is enhanced first by MEG alone, and then by the combined effects of MEG and the onset of biexciton binding [6].



**FIGURE 1.** Topology of the dominant character of single particle electron/hole states in the ground state bi-exciton.

## REFERENCES

1. V.I. Klimov, *Appl. Phys. Lett.* **89**, 123118 (2006)
2. F.C.M. Spoor, S. Tomić, A.J. Houtepen, L.D.A. Siebbeles, *ACS Nano* **11**, 6286 (2017)
3. J. Kim, L.-W. Wang, and A. Zunger, *Phys. Rev. B* **56**, R15541(R) (1997).
4. L. Bernasconi, S. Tomić, M. Ferrero, M. Rérat, R. Orlando, R Dovesi, *Phys. Rev. B* **83**, 195325 (2011)
5. E.J. Tyrrell and S. Tomić, *J. Phys. Chem. C* **119**, 12720 (2015)
6. S. Tomić, J.M. Miloszewski, E.J. Tyrrell, D.J. Binks, *IEEE J. Photovolt.* **6**, 179 (2016)
7. M.A. Leontiadou, E.J. Tyrrell, C.T. Smith, D.Espinobarro-Velazquez, R. Page, J. Miloszewski, T. Walsh, D. Binks, S. Tomić, *Sol. Energy Mater Sol. Cells* **159**, 657 (2017).
8. C.T. Smith, E.J. Tyrrell, M.A. Leontiadou, J. Miloszewski, T. Walsh, M. Cadirci, R. Page, D. Binks, S. Tomić, *Sol. Energy Mater Sol. Cells* **158**, 160 (2016).