STOCHASTIC SIMULATIONS OF THE SYNTHESIS OF NANOCRYSTALS IN REVERSE MICELLES

F. Mavelli[a], M.L: Curri[b], M. Striccoli[b], A. Agostiano[a,b]
[a]Dip. Chimica Università degli Studi di Bari, Via Orabona, 4 70126 Bari Italy
[b]CNR IPCF Bari Division, c/o Dip. Chimica Università degli Studi di Bari, Via Orabona, 4 /0126 Bari Italy
E-mail: mavelli@area.ba.cnr.it

In the past decade, semiconductor nanoparticles have attracted much attention arising from the fundamental scientific interest in understanding the transition of material properties from the bulk to molecular-like clusters and their potential applications. The main issue in the preparation of semiconductor nanocrystals is a careful control of particle size and, even more important, their size distribution. Among the several preparations proposed a popular method makes use of reverse micelles or water in oil microemulsions, undergoing to fast development in the last few years [1]. Nanoparticles can be obtained by using self-assembly molecules as a template, exploiting confined growth inside the surfactant film of microemulsion system. Stochastic simulation methods can be effectively exploited to account for the observed template effect of the microemulsion aggregate size on the nanocluster growth [2]. In this contribution a computer program that simulate the time evolution of this process will be presented and the obtained outcomes discussed. The program is based on the Gillespie algorithm [3], a Monte Carlo procedure that exactly simulate the master equation associated with any chemically reacting system. This approach allows to describes into details all the reactions that take place in the systems, i.e. solute exchange among droplets, nucleation and growth of nanocrystals, solute sedimentation. Moreover, the size dispersion of the reverse micelles can be taken into account. The aim of this work is to get insight in all the microscopic reactions linked to macroscopic properties of the reacting system than can be opportunely regulate to obtain nanocrystals with the desired sharp size distribution.

References:

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