

EXCITATION ENERGIES OF $Zn_{n}S_{n}$ NANOPARTICLES

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In this work we report on the excitation energies of ZnS nanoparticles, an area on intense research triggered by the recent successful synthesis of small ZnS clusters by BelBruno et. al. [1], and the accurate measurements of the optical excitation spectra of such a nanoparticles by Calandra et. al. [2].

We have investigated the most likely structural families [3,4] of the ZnS nanoparticles, namely, spheroids, bulk-like, cluster-tubes and rings.

The results presented in this work are two-fold. First, we show a comparison between the excitation energies and oscillator strengths of these structure families, providing basic information for further optical applications of these compounds. As an example, in Figure 1 the optical spectrum of $Zn_{26}S_{26}$ is given. Second, these results are confronted with the experimental data of Calandra [2]. We have found that the excitation energies of the spheroidal nanoparticles agree well with the experimental measurements, which lies in a range of 5.25-6 eV. The comparison of the excitation energies of different structure-families can be seen in Figure 2. Since due the ultra-small size of the experimentally synthesized nanoparticles most of their atoms must lie on the surface, we hypothesize that the surface reconstruction occurring during the relaxation yields surface motifs resembling those of our spheroidal species. This fully characterizes the surface structure of these nanoparticles, an information not available from experiments, yet.

References:

- [1] A. Burnin, E. Sanville and J. J. BelBruno, *J. Phys. Chem. A*, **109** (2005) 5026.
 [2] P. Calandra, A. Longo, and V. T. Liveri, *J. Phys. Chem. B*, **107** (2003) 25.
 [3] S. Hamad, C. R. A. Catlow, E. Spano, J. M. Matxain and J. M. Ugalde, *J. Phys. Chem. B*, **109** (2005) 2703.
 [4] J.M. Matxain, J. E. Fowler and J. M. Ugalde, *Phys. Rev. A*, **61** (2000) 512..

Figure 1: Optical spectrum of $\text{Zn}_{26}\text{S}_{26}$

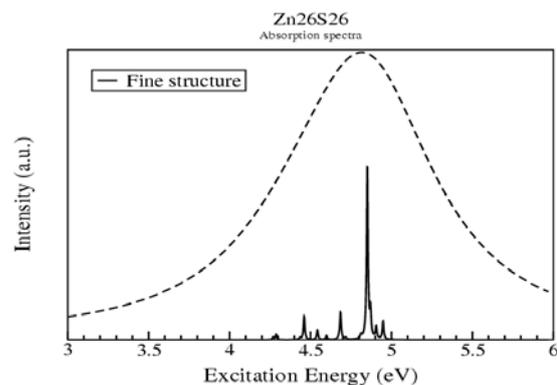
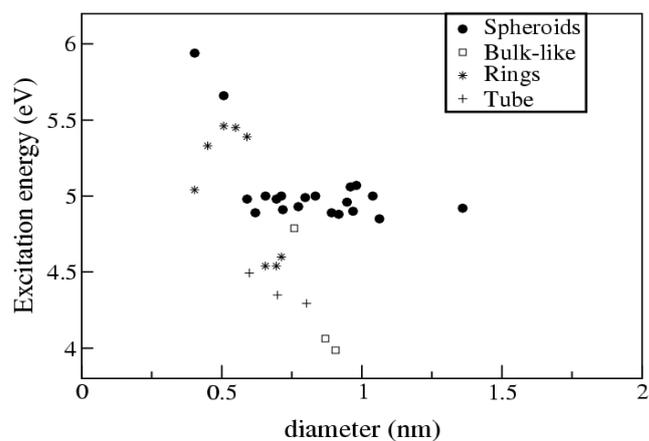


Figure 2: Excitation energies of different structure-families in function of the diameter of the



particle.