ENDOHEDRICAL (X@ZnnSn)^q Clusters, X=Li, Na, K, F, Cl, Br, n=4-16, q=0,1,-1

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Isolated neutral Zn_nS_n clusters, n=4-47 have been theoretically [1,2] studied in previous studies. The most stable structures were seen to be spheroid-like bubble structures, resembling carbon fullerenes. These structures have recently been synthesized experimentally, but in the cationic form [3].

The goal of the present work is two-fold: first, characterize the structure of the cationic and anionic isolated clusters, and then compare the results to the experimental ones [3]. Second, characterize the endohedric compounds of these cationic, neutral and anionic clusters.

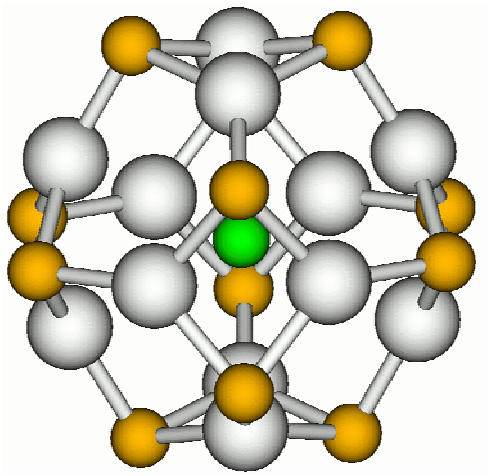
We have seen that both cationic and anionic clusters follow the same structural pattern, i.e. They are hollow bubbles built by squares and hexagons. Alkali metals and halogens have tested in order to check whether these clusters are able to trap atoms inside. We conclude that alkali metals are easier to be trapped in the center of the cluster than halogens. In Figure 1 the characterized Na@Zn12S12 is plotted. In Figure 2, the $Cl@Zn_{16}S_{16}$ structure is shown. It can be observed that while Na atom is trapped in the middle, Cl is linked to a Zn atom. We provide a full discussion of all characterized structures is done, and properties such as infrared spectra and structural properties are studied and compared to the isolated clusters.

References:

[1] S. Hamad, C. R. A. Catlow, E. Spano, J. M. Matxain and J. M. Ugalde, J. Phys. Chem. B, **109** (2005) 2703.
[2] J.M. Matxain, J. E. Fowler and J. M. Ugalde, Phys. Rev. A, **61** (2000) 512..
[3] A. Burnin, E. Sanville and J. J. BelBruno, J. Phys. Chem. A, **109** (2005) 5026.

Figures:

Figure 1: $Na@Zn_{12}S_{12}$



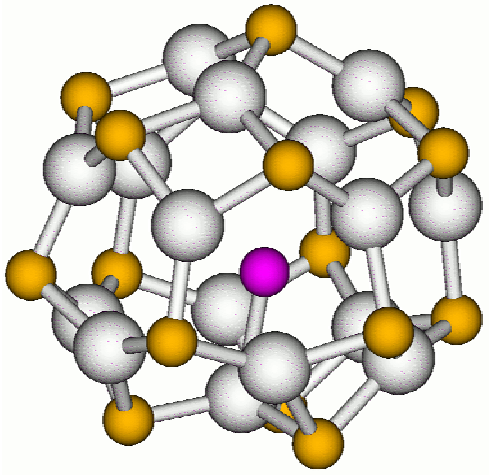


Figure 2: $Cl@Zn_{16}S_{16}$