

Molecular Polarizability of Sc Clusters and Endohedral Fullerenes

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The interacting induced dipoles polarization model implemented in the program POLAR (1) is used for the calculation of the molecular dipole-dipole polarizability α . The method is tested with Sc_n clusters and endohedral $Sc_n@C_m$ fullerenes (2-6). The polarizability is an important quantity for the identification of clusters with different numbers of atoms, and for the separation of isomers. The results for the polarizability are of the same order of magnitude as reference calculations carried out with the program PAPID (Fig. 1). In general, the inclusion of charge transfer modifies the result in the correct direction. The bulk limit for the polarizability is estimated from the Clausius-Mossotti relationship. The polarizability trend for these clusters as a function of size is different from what one might have expected. The clusters are more polarizable than what one might have inferred from the bulk. Previous theoretical work has yielded the same trend for Si_n , Ge_n and Ga_nAs_m small clusters. However, previous experimental work has yielded the opposite trend for Si_n , Ga_nAs_m and Ge_nTe_m larger clusters. At present, the origin of this difference is problematic. One might argue that smaller clusters need not behave like those of intermediate size. The high polarizability of small clusters is attributed to dangling bonds at the surface of the cluster. The clusters resemble *metallic* clusters. Provisional conclusions follow. (1) On varying the number of atoms, the clusters show numbers indicative of particularly polarizable structures. The polarizability is an important quantity for the identification of clusters with different numbers of atoms, and even for the separation of isomers. (2) The $\langle \alpha \rangle$ results are of the same order of magnitude as PAPID references. In general, the inclusion of charge transfer modifies $\langle \alpha \rangle$ in the correct direction. (3) The $\langle \alpha \rangle$ calculated with POLAR without charge transfer increases 18% from C_m to $Sc_n@C_m$, and with POLAR with charge transfer augments 2% from C_m to $Sc_n@C_m$. These results are rather underestimated when compared with PAPID without and with charge transfer. (4) The polarizability trend for the clusters as a function of size is different from what one might have expected. The Sc_n clusters (POLAR and PAPID), fullerenes (POLAR with charge transfer) and metallofullerenes (POLAR with charge transfer and PAPID with charge transfer) are more polarizable than what is inferred from the bulk.

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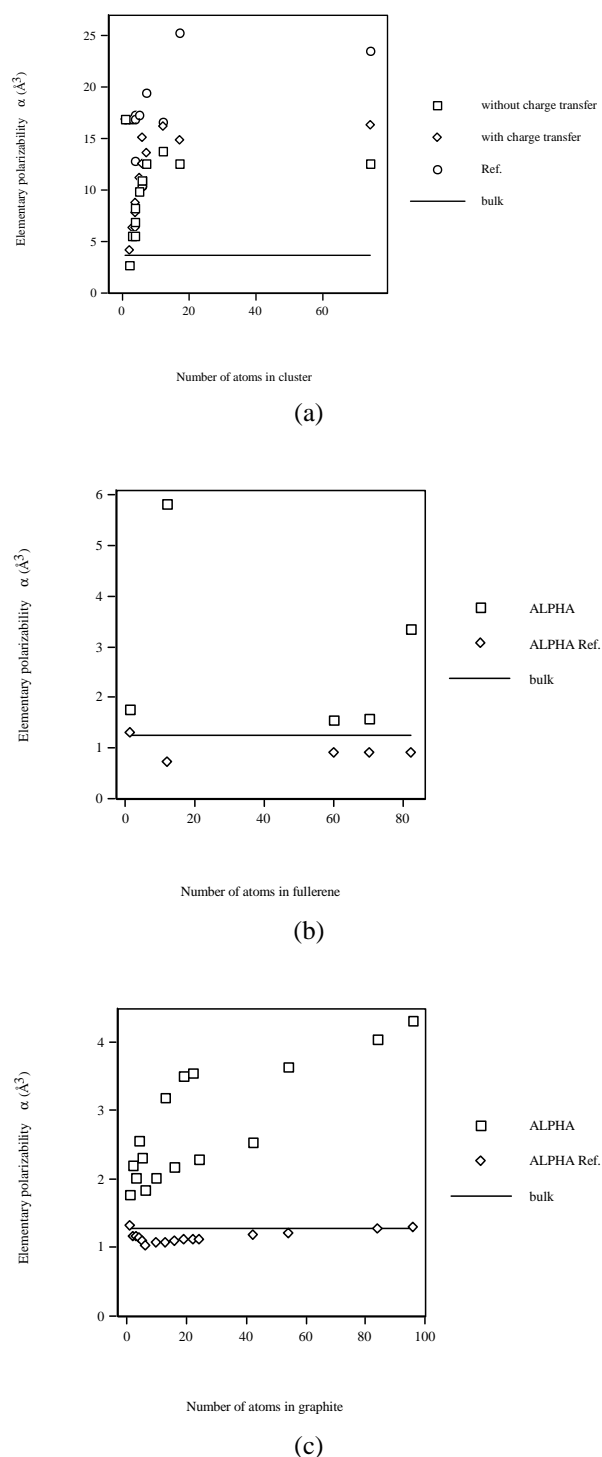


Fig. 1. Average atom-atom polarizabilities per atom of (a) Sc_n clusters, (b) fullerenes and (c) one-shell graphite models vs. cluster size. Dotted lines correspond to the bulk polarizabilities.