MONOPOLE-DIPOLE INTERACTION MODEL FOR CARBON ONIONS

N. Geuquet[1], R. Langlet[1], A. Mayer[1], L. Henrard[1] and Ph. Lambin[1]
[1]*Laboratoire de Physique du Solide, Facultés Universitaires Notre-Dame de la Paix, rue de Bruxelles 61, 5000 Namur, Belgium*
nicolas.geuquet@fundp.ac.be

We have modelled the dielectric response of fullerenes and carbon onions with a regularized monopole-dipole interaction model, which takes into account itinerant charges of the carbon sp^2 network [1]. The model has three adjustable parameters that were fitted to reproduce the measured polarizability values of isolated C_{60}, C_{70} and C_{84} molecules, essentially [2]. This model allows us to deal with the metallic behaviour of some carbon nanosystems. It yields a fairly good behaviour of the polarizability of fullerenes of various sizes and shapes. Calculations of static polarizability of hyper-fullerenes were performed with this model, for both single-shell and multi-shell nested hyper-fullerenes. This work aimes at characterizing the dielectric properties of nanocomposites materials embedding onions and onion-like carbons. (NATO Sciences for Peace Project 981051)

References

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