Calculations on Selected Charged Systems of Interest in Fullerene-Based Superconductivity

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Since the discovery of the fullerene-based superconductivity in K_3C_{60} with the critical temperature T_c of 18 K (A. F. Hebard *et al.*, Nature **350** (1991) 600) fullerene derivatives have been of focused interest of the superconductivity research. Although there is no generally accepted theory of the fullerene-based superconductivity, quantum-chemical computations can be of a considerable use in the research (Z. Slanina and S.-L. Lee, Chin. J. Phys. **34** (1996) 633). The usage is, for example, related to two well working empirical correlations of the fullerene-based superconductivity with the material properties. One is based on the fact that some Raman spectral shifts in A_xC_{60} mixtures are related to stoichiometry x (only $x = 3$ is superconductive and the stoichiometry can simply be deduced from the vibrational shift). The other correlation is a linear relationship between the lattice constant of A_3C_{60} and its critical temperature T_c. The lattice constant can also be deduced from quantum-chemical computations. Hence, quantum chemistry can serve as an alternative source of molecular parameters, especially in screening new materials. In addition to that, charge distributions are of some importance in reasonings on the fullerene-based superconductivity, and the charge distributions can be produced by quantum-chemical calculations as well. Very recently, fullerene-based superconductivity has been reported at much higher transition temperatures (even T_c of 117 K) when C_{60} single crystals are intercalated with simple halogen derivatives of methane (J. H. Schön *et al.*. Science **293** (2001) 2432). The present report deals with computations of related systems like C_{60}^{6-}, C_{60} & $CHCl_3$ or C_{60} & $CHBr_3$. Various structural and charge-distribution aspects are discussed.