Nanoscale physics

Supermolecular approximation in the studies of linear and nonlinear electric properties of spatially confined molecules

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In the last few decades there has been a growing interest in studies of molecular systems under spatial confinement. It is worth emphasizing that the term "spatial confinement" refers mainly to the inclusion compounds (chemical objects trapped inside different molecular cages, such as nanotubes and fullerenes) as well as matter under high pressure. It is well-established that the properties of spatially limited atoms and molecules can differ significantly from those in free space [1,2]. Therefore, such systems can contribute to development of many fields of science, including nanotechnology, spectroscopy, photonics, astrophysics, etc. In this context linear and nonlinear electric properties are of particular importance.

The purpose of this study is to analyze the influence of spatial confinement on the dipole moment, polarizability and first hyperpolarizability of the selected molecules (LiH, OCS, CO and BF) using supermolecular approximation, which is, next to the external analytical potentials, the most commonly used technique in quantum chemical studies of spatial confinement. To represent the chemical confining environment, various number of helium atom probes, at different orientations and distances from the investigated molecules, are used. Such approach allows to distinguish the orbital compression effect among other factors, which affect the electric properties of spatially restricted molecules. Our results demonstrate that the investigated electric properties strongly depend on the topology of the confining environment.

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