Nanoscale physics

On the importance of theoretical studies of the spatially confined atomic and molecular systems

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Nowadays, there is an increasing interest in the studies of spatially confined atomic and molecular systems, which is strongly connected with developments observed in nanotechnology over the last few decades. The classic examples of the spatial confinement phenomenon are inclusion compounds (chemical objects trapped inside molecular cages of different topology, such as nanotubes and fullerenes), artificial atoms and matter under high pressure. The spatial restriction can significantly modify various chemical and physical properties of atomic and molecular systems, including their electric properties [1]. It should also be noted that the experimental studies of spatially confined chemical objects are very challenging task, therefore, the quantum chemical investigations of such systems may stand as a relevant source of information.

The main goal of this work is to present the importance of the theoretical studies of the spatial confinement phenomenon. In doing so, we analyze the influence of spatial restriction on the electronic and vibrational contributions to the linear and nonlinear electric properties as well as two-photon absorption process of various atomic and molecular systems. The external spatial confinement is modeled by applying the harmonic oscillator potential. Such potential, added to the Hamiltonian of an isolated system in the form of one-electron operator, acts only on the electrons and accounts mainly for the effects arising from the Pauli exclusion principle. Therefore, the spatial confinement represented in such a way may correspond to non-polarizable, electronically inert environments [2,3].

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