

Two-photon absorption of the spatially confined LiH molecule

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The studies of spatially confined atomic and molecular systems have become a topic of great significance during the past few decades and increasingly attract attention of researchers from many fields of science. It is well-established that spatial restriction can strongly affect various physical and chemical properties [1-4]. In particular, much effort has been devoted to the studies on the electric properties of atoms and molecules in the presence of confining environment. However, it should be pointed out that previous work in this field has almost exclusively focused on the evaluation of the nonresonant electric dipole properties of molecular systems within restricted spaces, neglecting the nonlinear optical processes in the resonant regime. Therefore, our main goal is to investigate the two-photon dipole transitions between the $X^1\Sigma^+$ and $A^1\Sigma^+$ states of the LiH molecule in the presence of the confining environment. In doing so we consider the values of second-order transition moment. Additionally, we analyze the bond-length dependence of the two-photon absorption strength. The external spatial confinement is assumed in the form of cylindrically symmetric harmonic oscillator potential, which mimics a nanotube-like confining cages. The obtained results demonstrate that the spatial confinement can substantially influence the two-photon absorption response of LiH. In order to explain the observed changes in the second-order transition moment the two-level model is employed. The calculations are performed using multiconfiguration self-consistent field (MCSCF) method and response theory.

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