

The molecular electric properties under the influence of spherical harmonic potential

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Among many potentials that can be used to model the effect of spatial confinement the harmonic oscillator potential is one of the most widely applied. It allows for the representation of chemical cages of different structure, especially the nanotube-like or fullerene-like ones. It is important to note that in the vast majority of works devoted to the studies of electric properties of spatially confined systems, the harmonic potential of cylindrical symmetry was applied [1-3]. Thus far, its spherical counterpart was used mainly to describe properties of spatially restricted atomic systems [4-5]. Therefore, our main goal was to analyze how the presence of the spherically symmetric harmonic oscillator potential affects the molecular electric properties and to characterize the impact of the relative position of the considered molecules and spherical confinement on these properties. Moreover, we made an attempt to assess the influence of the topology of confining environment on the dipole moment, polarizability and first hyperpolarizability, by comparing the results obtained in the spherical and cylindrical harmonic potential. The quantum-chemical calculations were carried out for three molecules with linear symmetry, i.e. LiH, LiF and HF. The conducted research demonstrated that the values of electric properties strongly depend on the relative position of the molecules and applied spherical harmonic potential. The trends of changes in the electric properties, caused by increasing the confinement strength, were found to vary quite significantly. Moreover, in the vast majority of cases, significant differences in the values of electric properties, obtained in the cylindrical and spherical confinement of a given strength, were observed [6].

References

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