Quantum Chemistry of Confined Systems:

Spectral Properties of Atoms and Molecules

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Advances in semiconductor technology during the last two decades has allowed to create very small spatial structures, so called quantum dots and wires, for which the quantum structure is resolvable. Quantum dots, also known as artificial atoms, may be modelled by confining electrons into an external potential. Similarly, foreign atoms and molecules embedded into liquid helium and helium droplets, into fullerenes and into zeolites may be modelled by confining atoms and molecules into an appropriate external potential. A review about theoretical studies of spatially confined quantum systems has been given by Jaskólski [1]. A rather complete list of recent studies of spatially confined atoms has been published by Connerade [2]. Most of these studies are concerned with one-electron systems or with many-electron atoms described at the Hartree-Fock level. Very little is known about the influence of the electron correlation and the form of the confinement on the properties of confined system.

We have applied standard quantum-chemical models like the Hartree-Fock (HF), the configuration interaction (CI) and the couple cluster (CC) method to study the effects of spatial confinement of the atoms and molecules. The confinement is modelled by an external one-particle potential. The calculations are performed using, among others, the OpenMol Program [3]. We have studied the atoms and molecules $He, Li, Be, B, Ne, H_2, LiHandLi_2$ in spherical and non-spherical (ellipsiodal) power potentials and in center and off-center position. In particular, we analyse the spectral properties of the atoms and molecules as function of the different forms of confinement

References

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