

# Preface

Due largely to their relevance in the design and synthesis of new materials and futuristic devices, quantum confined model systems incorporating the repulsive as well as attractive confining potentials have become a subject of growing research interest. A diverse set of experiments involving, e.g. atoms and molecules under pressure, quantum dots and atoms in metallofullerenes are analysed using such models which are essentially defined by the given shape and strength of confining potential. Comprising a set of nine contributed chapters, dealing with the simplest among the quantum confined model systems, this monograph records the significant developments in the field subsequent to the two published volumes of *Advances in Quantum Chemistry* (Academic Press, New York, 2009), Vol. 57–58. In Chap. 1, Eugenio Ley-Koo and Guo-Hua Sun present their work on surface effects in light atoms confined by dihedral angles in spherical, parabolic and prolate spheroidal coordinates. In Chap. 2, Vladimir Pupyshev and Andrey Scherbinin discuss the effect of symmetry lowering of the confining impenetrable cavity, including the deformation of large cavity on the eigen-spectrum of hydrogen atom. In Chap. 3, Norberto Aquino and A. Flores-Riveros discuss their work covering the effect of soft spherical confinement on the popular information theoretical measures due to Shannon and Fisher for the hydrogen atom in the position and momentum space. In Chap. 4, H.E. Montgomery Jr. and K.D. Sen present the accurate total energy calculations on the two electron isoelectronic systems in excited electronic states within the impenetrable spherical boundary wall using variational perturbation method. The following Chap. 5 contributed by Frederico Prudente and Marcilio Guimarães describes the finite element and discrete variable representation under the variational ansatz for the treatment of the few electrons under the spherical, endohedral and plasmatical confinement conditions. Chapter 6, by L.G. Jiao and Y.K. Ho, presents a set of highly accurate calculations on the bound and resonant states in confined quantum dots. In the contribution under Chap. 7, S.A. Ndengué and O. Motapon use the Galerkin variational method with the wave functions obtained as expansions on B-splines basis sets in spherical, cylindrical or prolate spheroidal coordinates. The authors describe how the electronic energy levels of hydrogen atom, its wave functions and static and dynamic electric dipole

polarizabilities are significantly changed under the spherical, cylindrical or prolate spheroidal, endohedral or shell confinement conditions. The latter model potential is frequently used to model the confinement effects arising from a single and multi-wall fullerene cage. The study is extended to the investigation of the  $\text{H}_2^+$  molecular ion and its isotopologues. In Chap. 8, J. Garza and R. Vargas formulate the scheme of carrying out the Thomas-Fermi, modified Thomas-Fermi and the density functional theory (DFT) calculations within the Kohn-Sham model for the spherically confined many electron atoms. The influence of confinement on the correlation energy has been studied within the DFT. Finally, in Chap. 9, A. Sarsa and C. Le Sech study the effect of quantum confinement on the  $\text{H}_2^+$  molecular ion and  $\text{H}_2$  molecule. For these molecules confined by impenetrable surfaces the trial wave functions are computed using the variational and diffusional Monte Carlo approaches. The study is carried out beyond the Born-Oppenheimer approximation so that the motion of the nuclei is included in the trial wave function. It is hoped that the theoretical formulations, algorithms and their applications contained in this monograph will serve as a ready reference material to the interdisciplinary research community interested in studying confined quantum electronic systems.

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