Amlan K Roy et al., J Laser Opt Photonics 2019, Volume 06
DOI: 10.4172/2469-410X-C2-049



## Effect of spatial confinement on the electronic structure of atoms: A density functional formalism

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A many-electron system enclosed inside an impenetrable hard spherical cavity introduces many significant changes in the observable properties, such as energy spectrum, transition frequency, transition probability, polarizability, ionization potential, chemical reactivity etc. Thus, recently considerable attention has been paid to study these systems, both theoretically and experimentally. Quantum confinement is encountered in many different physical situations, e.g., atoms under plasma environment, impurities in crystal lattice and semiconductor materials, trapping of atoms/molecules in zeolite cages, quantum wells, quantum wires, quantum dots etc. This talk presents the development of a density functional theory (DFT)-based method for accurate and reliable treatment of quantum confinement in ground and excited states of atoms. Over the past four decades, DFT has achieved impressive successes in explaining the electronic structure of atoms, molecules and extended systems, and thus remains the favoured choice to probe such systems. However, a satisfactory treatment of excited states has remained a bottleneck, ever since the inception, even though several elegant and attractive formalisms have been proposed with time. In literature, there are reports of various wave-function based approaches (such as HF, CI, Hylleraas, Perturbative, Ritz-variational, POEP) to study atoms under various confining conditions. We adopt a physically motivated non-variational, work-function based exchange potential, along with some approximate local and nonlinear, gradient-corrected correlation functionals, to account for the subtle electron correlation effect. The resulting KS equation has been accurately and efficiently solved by means of a generalized pseudospectral (GPS) method which offers a non-uniform, optimal spatial discretization

6th World Congress on
Physics
May 13-14, 2019 | Paris, France

leading to a symmetric eigenvalue problem. A comparison with literature results reveals that our exchange-only results are as accurate HF method, while with correlation included; these are very competitive to the much more sophisticated and elaborate multi-configurational calculations. A detailed discussion is made on the effect of correlation on confinement. Additionally, some recent results of various information theoretical tools, like Shannon entropy, Renyi entropy, Tsallis entropy, Fisher information, Onicescu energy, etc., in ground and excited states of such systems, would also be presented. To conclude, the present method provides a computationally efficient and accurate scheme to study confined atomic systems within DFT.

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## Biography

Amlan K Roy has completed his PhD in Theoretical Chemistry from Panjab University, in India. Later he pursued his Post-doctoral research in a number of places in North America, such as University of New Brunswick (Fredericton, Canada), University of Kansas (Lawrence, USA), University of California (Los Angeles, USA), University of Florida (Quantum Theory Project). His primary research interest is to develop methods for electronic structure and dynamics of many-electron systems, within the broad domain of density functional framework. Presently he is an Associate Professor at IISER Kolkata. He has published more than 70 research papers and book chapters in reputed journals. He has been serving as a Reviewer in several renowned journals. His biography has been included in 63rd Edition of Marquis Who's Who in America, 2009. In 2012 he has edited a book entitled "Theoretical and Computational Developments in Modern Density Functional Theory".

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