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Confined Atomic Systems

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Abstract

In this thesis, we investigate physical properties of various atomic systems such as hydrogen, helium and argon confined in a soft-wall potential of the form $V_s(r) = (r/r_0)^N$, where r_0 is the radius of the spherical confinement and N is the stiffness controlling variable. Our main purpose is to introduce a confinement for atomic systems that is flexible in terms of stiffness of the confining walls. However, this brings its complications such as non-existence of analytic solutions to the non-relativistic Schrödinger equation for this particular problem, and non-availability of good basis sets for studying electronic properties of such systems. Therefore, at first, we treat the problem in pure numerical fashion. Based on our experience on the numerical data, we then attempt to design basis sets that can be used in quantum chemical software packages. We compare our results to known theoretical and experimental results and, in return, make a decision on the quality of the basis sets. To our knowledge, systems confined in this type of potential has not yet been studied, and, we believe that this study will open up new research areas in this field. Possible applications are in high-pressure simulations of atomic, or molecular systems.

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