



SDI Review Form 1.6

Journal Name:	Asian Journal of Chemical Sciences
Manuscript Number:	Ms_AJOCS_34565
Title of the Manuscript:	Direct property calculation of atom: A classical approach
Type of the Article	Original Research Article

General guideline for Peer Review process:

This journal's peer review policy states that **NO** manuscript should be rejected only on the basis of '**lack of Novelty**', provided the manuscript is scientifically robust and technically sound.

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PART 1: Review Comments

	Reviewer's comment	Author's comment (if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)
<u>Compulsory</u> REVISION comments	<p>This work has a very limited value. It is heavily dependent on some already-known values of energies and experimental radii. Even to determine various parameters, approximate values of energies of two electron systems have been used, instead of the exact known values.</p> <p>Moreover, when accurate values of energies are already available, chances of anyone using the presently calculated energy values is almost zero. It cannot be used to calculate any property of the system under consideration. It does not indicate corrections to the nonrelativistic energy. There is no indication how well the virial theorem is satisfied for the system, nothing can be known about the correlation and exchange energies.</p> <p>What is the value of the density in Eq. (6) for any particular atom? Is Eq. (2) used everywhere?</p> <p>It seems that the present method does not have any variational bound. Does it provide an upper bound on the results obtained from Eq. (6)? A much lower result of any energy could be obtained compared to the exact value.</p> <p>Perhaps, the authors would like to calculate energies of hydrogen molecular ions where accurate results have been obtained without separating the electronic and nuclear motions [for example, cf. A. K. Bhatia, Phys. Rev. A 58, 2787 (1998), and references therein]. Perhaps, for such systems, the authors could make a mark.</p>	<p>I am sorry to say that the present theory is completely different from what the reviewer assumed. It is a theory for electronic energy calculation and property calculation for atom with out any basis function or so called quantum formulation. There is no Hamiltonian. It uses only the concept of DFT not the exact DFT procedure. Is it not great to calculate IP of an atom with out using basis, Hamiltonian and any kind of computational facilities? As it is not a ab-initio quantum method there is no virial theorem, variational bound. Yes, the values reported may not be interested for others but, it is required for showing the accuracy of present method. This method would be very much useful if it is applicable for molecules. Present article is just one step towards that destination.</p>
<u>Minor</u> REVISION comments		
<u>Optional/General</u> comments	Revisions are needed	