



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.

To know the complete guideline for Peer Review process, reviewers are requested to visit this link:

(<http://www.sciencedomain.org/page.php?id=sdi-general-editorial-policy#Peer-Review-Guideline>)



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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)
Compulsory 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. 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>	
Minor REVISION comments		



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<u>Optional/General</u> comments	Revisions are needed	
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Reviewer Details:

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