SCIENCEDOMAIN *international*
www.sciencedomain.org

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)

SDI Review Form 1.6

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	**The author(s) proposed good correlation equations for calculation of total energy of the atoms and 1st ionization potential. Optimization of parameters led to accurate conformity with experimental and theoretical data, calculated by other methods. It may be useful for further calculations of molecules parameters and properties, although it is not clear how.** **But authors' appeal to classical mechanics is incomprehensible. They operate within quantum mechanics, namely density functional theory (DFT). And their aim (as I understood) is to facilitate calculations in the framework of DFT. So the words "A classical approach" should be excluded from the title, as well as from the abstract.** **Please clarify the ethical issue if any** The paper presented is the literal copy of the paper by Arijit Bag "Ground State Electronic Energy and Ionization Energy of Atoms: Basis Free Partitioned Classical Density Functional Theory (PCDFT) Calculation" issued in Journal of The International Association of Advanced Technology and Science, 2015, V. 16, No 3. I have no information about the author(s) of the reviewed paper and I suppose that it may be the same person (Arijit Bag), but in any case it is not cool. If it is Arijit Bag, editorial board should make the decision according to Journal's policy. By the way, the title of the "old"	

SDI Review Form 1.6

	paper was better.	
Minor REVISION comments	I am not sure that the data for Berkelium, Bk, and following (Table 1) are important. There we have no experimental data for comparison, so these data can be excluded. By the way, some elements from this list have acquired names recently.	
Optional/General comments		

Reviewer Details:

Name:	***Heinrich Ehrlich***
Department, University & Country	***Chemistry Faculty, Lomonosov Moscow State University, Moscow, Russia***