



SDI Review Form 1.6

Journal Name:	Asian Journal of Physical Sciences
Manuscript Number:	Ms_AJOPS_30695
Title of the Manuscript:	THE COHESIVE ENERGY CALCULATIONS OF SOME BCC (Li, Cr, Fe, Mo) LATTICES USING DENSITY FUNCTIONAL THEORY
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:

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PART 1: Review Comments

	Reviewer's comment	Author's comment <i>(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)</i>
<u>Compulsory</u> REVISION comments	<p>1) An English revision is very necessary in this manuscript, there are some mistakes even in the 'Abstract' section.</p> <p>2) The reason why that authors choose LDA in this paper has to be carefully explained.</p> <p>3) The cohesive energy of bcc lithium was calculated to be approximately 1.82eV which is in good agreement as compared to experimental value of 1.63eV. This deviation seems to be acceptable. While, for the other three bcc Cr, Fe and Mo, the obtained results seems a little bigger than that of experimental values (about 25% exceed). How to explain the differences of the results?</p> <p>4) The crystalline structure of all the metals should be clearly provided and the number of atoms in each model have to be shown.</p>	<p>(1) to (3): All corrections effected.</p> <p>(4) Authors see that visuals of the metals will result to mere repetition of structures. Authors also see that bulk structures are inexpensive when their sizes become larger and larger in terms of total energy. However authors may consider this kind of approach in subsequent articles.</p>
<u>Minor</u> REVISION comments		
<u>Optional/General</u> comments		