



**SDI Review Form 1.6**

Journal Name:	<a href="#">Asian Journal of Physical Sciences</a>
Manuscript Number:	<b>Ms_AJOPS_30695</b>
Title of the Manuscript:	<b>THE COHESIVE ENERGY CALCULATIONS OF SOME BCC (Li, Cr, Fe, Mo) LATTICES USING DENSITY FUNCTIONAL THEORY</b>
Type of the Article	<b>Original Research Article</b>

**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)
<b>Compulsory</b> REVISION comments	<p>1. The authors used a <b>very powerful code</b> (FHI-aims) to <b>solve a rather simple problem</b>: to calculate cohesive energies of simple crystals – Li, Cr, Fe, Mo. Why?</p> <p>2. The authors state in details the well-known density functional theory and the Kohn-Sham approach so, as if they are new. I think to it would be sufficient to make citations.</p> <p>3. The authors do not specify what parameters of lattices they use in calculations. They don't report, whether they find their equilibrium values.</p> <p>4. The authors study magnetic crystals (Fe and Cr) without spin-polarization. Why?</p> <p>5. The authors demonstrate increasing of the total energy of crystals at increase in number of iterations instead of its decrease. It is a nonsense!</p> <p>6. Changes of a total energy in the course of iterations are so small that the values of cohesion energy given by authors can be received on the first iteration. It is very strange.</p> <p>7. The authors do not compare their results with values calculated other researches. For example, for Mo there is a work (PRB 47, 1993, 2979) where data obtained by different methods are compared). Authors can easily find such papers for Li, Cr and Fe.</p>	<p>1. Authors have used FHI-aims code to calculate structural properties (cohesive energy) of the crystals because it provides information on binding strength, structural preferences and research data of the solids. Authors are aware of the power of FHI-aims and intend to delve into other areas using the code in subsequent articles.</p> <p>2. Authors only tried to explain the concept of DFT and the KS approach in simple forms. Nonetheless, the reviewer's comment is noted.</p> <p>3. Noted. That correction has been effected on the revised manuscript in tabular form.</p> <p>4. There was spin treatment of Fe and Cr in the input setting (control. in) of the FHI-aims code. The spin treatment is set to 'collinear', which requests a spin-unrestricted (polarized) calculation. Explicit spin-unrestricted calculation was done for the ferromagnetic crystals, Fe.</p> <p>5. Noted, but total energy increase at the beginning is not continuous to the end of the iterations. Anyway, authors will reframe: the total energy for Li bulk tends towards stability as the number of iterations increases.</p> <p>6. That may have come from the code's default settings of Self-Consistent field (S.C.F) for accuracy.</p> <p>7. These corrections have been effected.</p>
<b>Minor</b> REVISION comments		
<b>Optional/General</b> comments		