



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:

(<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)
<u>Compulsory</u> REVISION comments	<p>1. The authors used a very powerful code (FHI-aims) to solve a rather simple problem: 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>	
<u>Minor</u> REVISION comments		
<u>Optional/General</u> comments		

Reviewer Details:

Name:	Anonymous
Department, University & Country	Institute of Materials Science, Russia