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SDI FINAL EVALUATION FORM 1.1

PART 1:

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 Article:	**Original Research Article**

PART 2:

FINAL EVALUATOR'S comments on revised paper (if any)	**Authors' response to final evaluator's comments**
3. Authors didn't compare their equilibrium values for lattice constants with experimental and other ones. They must do that. 4 OK about Fe, however it must be clear marked in the test. 5. It seems to me the authors even don't understand the main trouble of their paper. They calmly demonstrate increasing of the total energy of crystals at increase in number of iterations instead of its decrease. This is physically impossible. 6. This result demonstrates that the authors made something PRINCIPAL wrong in calculations. No one code can provide such results. ********** If the 5 and 6 items will not be revised the paper can not be published.	3. Authors used experimental values of lattice constant which is certainly inexpensive (usually about 1% difference from equilibrium lattice constants); however, they may do as evaluator suggested in other future work. 4. OK 5. Authors see that there is no trouble as long as total energy does not increase towards the end of iterations, but converges. Authors can say here that the converged values for total energy of crystals or bulk structures are decreased or less than those of their corresponding atoms as shown clearly in table 1 of the revised manuscript. 6. If there was error in calculations, FHI-aims codes would point it out clearly or calculations would stop running, and you wouldn't find the line " Have a nice day" signifying convergence of calculations. Authors see that what is important is that total energy converges at least and can be clearly seen as shown in the graphs; and total energy corrected for atom and bulk structures of all the metals are used to calculate the cohesive energies. Also, authors have claimed that the small changes observed in total energy may have come from the code's self-consistency field (S.C.F.) settings for accuracy in iterations. Finally, authors see that what they expected from their investigation, that is, cohesive energy values were calculated in the neighbourhood of experimentally found values and results from others.