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SDI Review Form 1.6

Journal Name:	**Physical Science International Journal**
Manuscript Number:	**Ms_PSIJ_29954**
Title of the Manuscript:	**Free energy estimation of a binary alloy around the equilibrium based on the order parameter**
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** *(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		
Minor REVISION comments	**Introduction** When we read "atoms of type A and NB atoms of type B [1]. (figure 1)", we must read "atoms of type A and NB atoms of type B [1] (figure 1).". When we have card Ω, it is important to mention that "card Ω" represent the "number of elements of the set". For other hand card Ω is not the same of Ω, because Ω is "space of the possible positions" and card Ω is "the number of permitted configurations". The equality card Ω=Ω is wrong.	Thank you for your comments; we will take them into account. For about card Ω your are right, we mean cardΩ=|Ω|, it's just a latex typo error, we will correct it.

	After present the equation 1.1 it is necessary to mention that S represents the entropy. **b) Free Energy formula** It is important mention that in the formula F=U-TS, that U is the internal energy of the system and T the absolute temperature of the surroundings. When we read "With ….. In the regular case, the entropy always", we word "With" must start with lowercase letter. When we read "The probability lows of atoms", we must read "The probability laws of atoms". In the equation 1.3 it is important to identify the meaning of the P letter (probability). **2a) Free Energy formula based….** When we read "For the physicists, it is interesting to study the variation of this energy. Because, the equilibrium….", we must read	For S and U that's ok we will mention them at the beginning with the system data. For T we have already mentioned it at the beginning. In the beginning of line we start with a uppercase letter. P is already mentioned in the data system at the beginning. P_{XY}: the probability for which an atom of type X has a neighbor of type Y. That's ok.

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	"For the physicists, it is interesting to study the variation of this energy, because the equilibrium…". When we consider the simplification of equation 2.2, why, in such simplification, the author or authors consider that the term $-K_b T \frac{n}{\frac{1}{4}-n^2}$ is zero? Why the term $K_b T ln(\frac{\frac{1}{2}-n}{\frac{1}{2}+n})$ is zero? Why the term $K_b T n \frac{1}{(\frac{1}{2}-n)(\frac{1}{2}+n)}$is zero?	For this comment: $K_b T n \frac{1}{(\frac{1}{2}-n)(\frac{1}{2}+n)}$ and $-K_b T \frac{n}{\frac{1}{4}-n^2}$ are two opposite quantities so their sum is equal to zero. The term $K_b T ln(\frac{\frac{1}{2}-n}{\frac{1}{2}+n})$ is not equal to zero it appears in the equation. You can find the steps calculus in follow: (If you want we can add these steps as annex in the paper). As you may know: $\frac{dE(\eta)}{d\eta} = \frac{d}{d\eta}\left[E_0 + z\left(\frac{1}{4}-\eta^2\right)\varepsilon + k_B T\left[\frac{1}{2}\ln\left(\frac{1}{4}-\eta^2\right) + \eta\ln\left(\frac{\frac{1}{2}+\eta}{\frac{1}{2}-\eta}\right)\right]\right]$ 1) $\frac{dE_0}{d\eta} = 0$ 2) $\frac{d}{d\eta}\left[z\left(\frac{1}{4}-\eta^2\right)\varepsilon\right] = -2z\varepsilon\eta$ 3) Let us consider the following term and develop it: $\frac{1}{2}\ln\left(\frac{1}{4}-\eta^2\right) + \eta\ln\left(\frac{\frac{1}{2}+\eta}{\frac{1}{2}-\eta}\right) = \frac{1}{2}\ln\left[\left(\frac{1}{2}-\eta\right)\left(\frac{1}{2}+\eta\right)\right] + \eta\ln\left(\frac{1}{2}+\eta\right) - \eta\ln\left(\frac{1}{2}-\eta\right)$ $= \frac{1}{2}\ln\left(\frac{1}{2}-\eta\right) + \frac{1}{2}\ln\left(\frac{1}{2}+\eta\right) + \eta\ln\left(\frac{1}{2}+\eta\right) - \eta\ln\left(\frac{1}{2}-\eta\right)$ Then its derivative is as follow: $\frac{d}{d\eta}\left[\frac{1}{2}\ln\left(\frac{1}{2}-\eta\right) + \frac{1}{2}\ln\left(\frac{1}{2}+\eta\right) + \eta\ln\left(\frac{1}{2}+\eta\right) - \eta\ln\left(\frac{1}{2}-\eta\right)\right]$ $= \frac{1}{2}\cdot\frac{-1}{\frac{1}{2}-\eta} + \frac{1}{2}\cdot\frac{1}{\frac{1}{2}+\eta} + \ln\left(\frac{1}{2}+\eta\right) + \eta\cdot\frac{1}{\frac{1}{2}+\eta} - \ln\left(\frac{1}{2}-\eta\right) - \eta\cdot\frac{-1}{\frac{1}{2}-\eta}$ $= -\frac{\eta}{\frac{1}{4}-\eta^2} + \frac{\eta}{\frac{1}{4}-\eta^2} + \ln\left(\frac{\frac{1}{2}+\eta}{\frac{1}{2}-\eta}\right)$ We have: $-\frac{\eta}{\frac{1}{4}-\eta^2} + \frac{\eta}{\frac{1}{4}-\eta^2} = 0$. So, $\frac{d}{d\eta}\left[\frac{1}{2}\ln\left(\frac{1}{2}-\eta\right) + \frac{1}{2}\ln\left(\frac{1}{2}+\eta\right) + \eta\ln\left(\frac{1}{2}+\eta\right) - \eta\ln\left(\frac{1}{2}-\eta\right)\right] = \ln\left(\frac{\frac{1}{2}+\eta}{\frac{1}{2}-\eta}\right)$ Therefore, $\frac{dE(\eta)}{d\eta} = -2z\varepsilon\eta + k_B T\ln\left(\frac{\frac{1}{2}+\eta}{\frac{1}{2}-\eta}\right)$

	3.1 Approximation Please denote also, in the condition following the equation 3.2 that k $\in \boldsymbol{N}$.	That's ok.
	b) Justification order choice When we read "therefor the minimum in", we must read "therefore the minimum in".	That's ok.
	Please correct the expression $\lim_{n_n \to n_0} E_4(n_n) + P(n_{n)}$ for $\lim_{n_n \to n_0} \left[E_4(n_n) + P(n_{n)}\right]$. The two terms are between parentheses.	That's ok.
	If P is a function of η, a single variable, what the author or authors want to say with "Thus, the unique critical point of P is (0; 0)."? What is the vector (0;0)? Means that P is zero when η is zero? If is that, please say it clearly.	Yes when η =0, P(0)=0, and because of P'(0)=0 when η =0 so the point (0,P(0)) is a critical point, means that the minimum of P is 0 in η =0 and the point that represents the minimum is (0,0). (0,0) is not vector it's a point.
	When we read "therefor P is strictly convex", we must read "therefore P is strictly	Ok.

	convex". **c) Study for the 4-th order case** When we read "Let un put," what that meant? Is "Let me put"? On the equation 3.21 from where comes the term $\frac{-F_1}{2F_2}$? Or the term $\frac{-F_1^2}{4F_2}$?	It means let us, typo error. Let us consider the equation (3.19), it's a derivative of E_4. As you may know the critical points that's to say the roots of this equation represent the minimum of E_4. (3.19) has two roots either η =0 or $F_1 + 2F_2\eta^2$ =0 that's to say $\eta_1 = \sqrt{\frac{-F_1}{2F_2}}$ or η_2 =-- $\sqrt{\frac{-F_1}{2F_2}}$, (! in this part we'we worked in the interval [0,1/2[that's why we'we took just $\sqrt{\frac{-F_1}{2F_2}}$), if $F_1>0$ there is no roots of $F_1 + 2F_2\eta^2$ so η =0 is the unique root of (3.19). But if $F_1<0$ we have 2 roots η =0 or $\eta_1 = \sqrt{\frac{-F_1}{2F_2}}$. Therefore the minimum of E_4 is in $\eta_1 = \sqrt{\frac{-F_1}{2F_2}}$, we've replaced η_1 in (3.18) we've founded $\frac{-F_1^2}{4F_2}$. Consequently the equation (3.21)

	What is the vector $(0, F_0)$? An equilibrium point in the space E, F? E is only function of η. Please precise mathematically the sentence.	$(0, F_0)$ is a point that means $(0, E_4(0))$ or clearly $E_4(0)= F_0$ In that point we find the minimum of E_4 or the equilibrium of the system.
	Remark 3.1 When we read "signs, nay their values", we must read "signs, not their values".	We meant even or also not not.
	References The references need a revision in order to have all important elements: Author family name, date, title, Editor and place of edition.	

Optional/General comments	Seems to me, to be important to clarify the mathematical steps of the expressions and the assumptions such as where the Taylor series is centred or the choices of the values of Tc. Seems to me also important to make a small description, elucidating about the big differences, of the figures 2 to 12.	