

Reviewers comments	Corrections
<p>Major comment: The paper requires major language editing. I recommend that the authors go through the text again and scrutinise the document very carefully. Alternatively, the authors might want to approach their Institution's language editing support services. There are far too many language related issues to list in this review report. Recurring mistakes include the mixing of singular and plural, e.g. in line 2 of page 5 "... the nanoparticles assumes a well-ordered cubic shapes ...". There are also many superfluous or missing punctuation marks and poorly structured sentences. The poor language use can lead to incomprehensible statements (e.g. in line 7 or the Introduction: "..., and high freedom for the volume change"). There are also a lot of sentences that do not contribute information, and should be taken out (e.g. the last sentence of the Abstract).</p>	<p>Major comments have been corrected accordingly.</p>
<p>Figure 1 caption: there should not be any indent in the first line.</p>	<p>Rectified</p>
<p>First seen in Line 7 of 2.1, but recurring many times throughout the paper, including in the equations: All variables like N, V, U, r, i, j, A, C, k, etc. should always be written in italics.</p>	<p>Changed and corrected</p>
<p>Line 7 in 2.1: Why is the type of thermostat specified? This work is a compilation of computational simulations, each specifically carried out under constant temperature conditions. If the type and characteristics of the thermostat affect the calculation, then it should be explained why. Otherwise that sentence can presumably be left out.</p>	<p>The specified thermostat is explained in the text.</p>
<p>Line 10 in 2.1: What is an "NP"? This acronym should be defined.</p>	<p>"NP" Removed</p>
<p>Equations 1, 2 & 3: The equation font size is too large. The font size should correspond to the rest of the text.</p>	<p>The equation font size changed accordingly.</p>
<p>Last line of 2.2.3: What is the "simulation of bulk and surfaces"? Presumably needs to be rephrased?</p>	<p>Rephrased</p>

<p>Lines 9-14 of 3.1: This is very cumbersome, and the text should never blandly repeat what is already illustrated in the graphs. This set of sentences should be restructured. Perhaps consider adding a column or two in Table 1 where all this information can be displayed more orderly.</p>	<p>Changed the paragraph</p>
<p>Same section as in previous point, and Fig 2: I am really not convinced of the evidence from the graph for energy changes below 1200 K. If a case can be made then this should be backed by further argumentation. Otherwise one can perhaps mention that there might be these features in the graphs, but that further calculations are necessary to confirm or refute these.</p>	<p>Paragraph was changed and explained differently</p>
<p>Section 3.2, paragraph 1: This section needs to be reworked to make it clearer and to the point. For example, to say that something “has a well-defined structure” is very vague. In a similar vein, convoluted phrases such as “suggestive of the liquid phase” or “temperatures leading to the melting” should be avoided in scientific writing. Same for “arrangement of atoms vanish” in the following paragraph.</p>	<p>Reworked the whole paragraph</p>
<p>Page 5: The line spacing in paragraph 2 of 3.2 and the Conclusion must be the same as for the other sections. All references must be spaced equally.</p>	<p>Changed accordingly</p>
<p>References: There are formatting inconsistencies. [5] must include an “and” before the last author, and no commas after that. The journal name in [15] must be in italics. In [18] there is an “:” that should be removed, and the last letters of the journal name must be in italics.</p>	<p>Changed accordingly</p>