

## Response to the comments

1. Reviewer comment #5, the Figure 1 was generated as it is from the calculation results. The legend was also given as it is from the output generated.
2. Reviewer comment #6, the sentence “This showed that that the cluster expansion represents the interactions of Pt-As-S more accurately have been removed since it is incomprehensible.
3. Minor comment #9, the supercell sizes were given in section 3.4 where there are all 2x2 supercell of PtAs<sub>2</sub>, PtAsS and Pd<sub>2</sub>As (100) surface.
4. Minor comment #10, adding the sentence “However, in Figures 3(b) and (c) the scale of the graph goes to -1, which suggests that the frequencies do actually go negative” contradicts with the previous sentence. The sentence indicate instability and all the PtAs<sub>2</sub>, PtAsS and Pd<sub>2</sub>As structures are stable and this has been proved by the calculated elastic constants.
5. Review comment #7, the input parameter used are the calculated surface energies in Table 2 above and it is indicated in section 3.5.
6. Minor comment #3, last comment in the conclusion. The conclusion cannot be referenced.

Letter to the Editor

Dear Editor

I have now addressed all the previous major and minor comments on the paper. All the corrections have been amended where necessary. The new comments are also addressed in full. The changes were made following the comments from the reviewers.

Regards

Nemutudi Bradley