# Is TPSS an TPSSh better for TPAA calculations?

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## 1 Introduction

Mention big picture -> lissoclimide project; follow-up to the previous report The TPSS and TPSSh functionals may describe the halogen-pi bond more accurately than PBE. To investigate which functional performs better, the X40 test set serves as a benchmark for TPSS, TPSSh, and PBE calculations.

## 2 Methods

Most of calculations are based on the previous report. The 3-4 extrapolation of the RIRPA correlation energy was good balance between efficiency and accuracy... The X40 Test Set was used the benchmark the method's accuracy for noncovalent interactions involving halogens remind your reader of the x40 test set - descriptions: type of interactions, and how many complexes. Calculations were computed with basis sets def2-QZVP, cc-pVTZ, and cc-pVQZ. The RPA energies were computed based on converged orbitals from TPSS and TPSSh and resolution of identity (RI) was included to improve efficiency.

For the sake of time, a set of eight complexes from X40 test set was chosen to study basis set convergences based on error from a previous report.

## 3 Results

Adding figures - lookup how to add figures; see Fig. 1 as good example

yada yada see Fig. 14 This section states the main new results of the current reporting period. These results could be presented, e.g., in the form of equations, figures, tables, and text. Negative results are just as important as positive ones and should be carefully reported. Use a balanced tone avoiding over- and understatement.

Sometimes, it is helpful to separate statement of the results and discussion, although a strict separation of the two is often impossible. A separate discussion section may be appropriate if you are proposing a speculative rationale or if several interpretations of your results are possible. If you have no new results at all, this is the place to explain why.

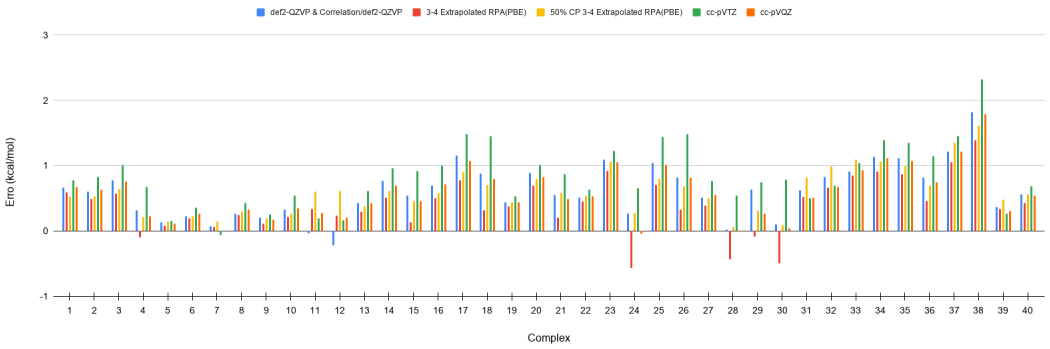



Figure 1: The binding energy errors (kcal/mol) for X40 test set computed for PBE, PBE-D3, PBE-D4, RPA(PBE), and def2-QZVP. All methods were 50 CP corrected and negative sign indicates overbinding.

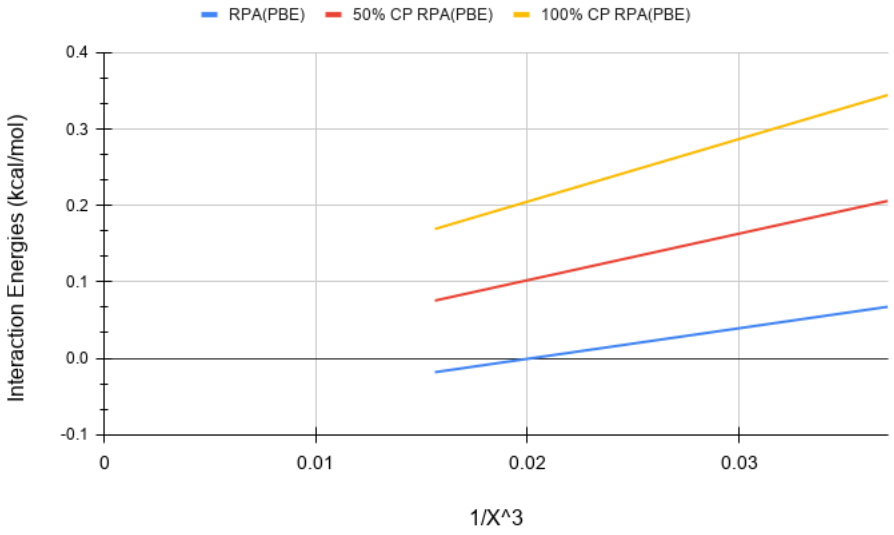
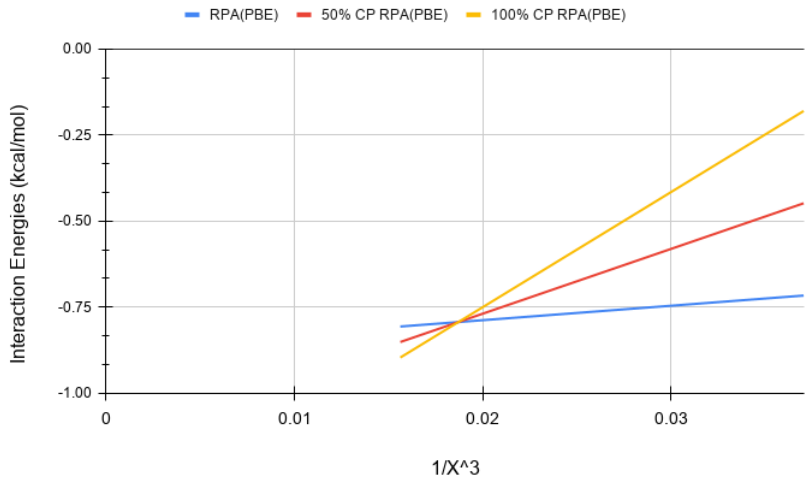
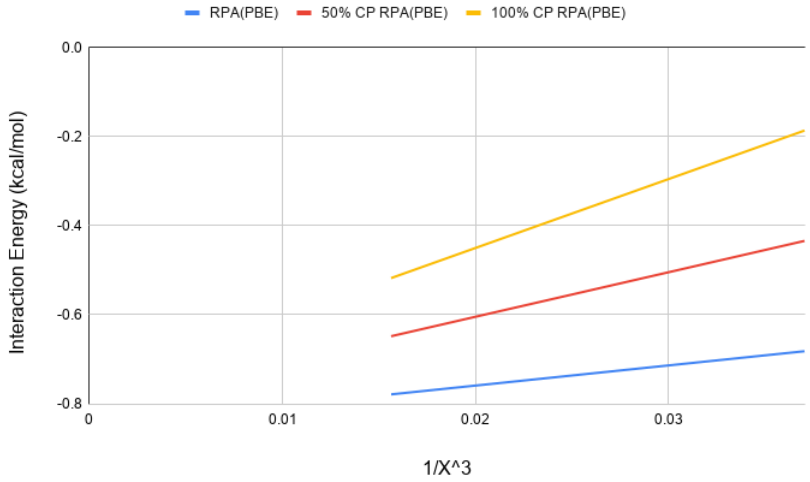



Figure 2: This is a figure.

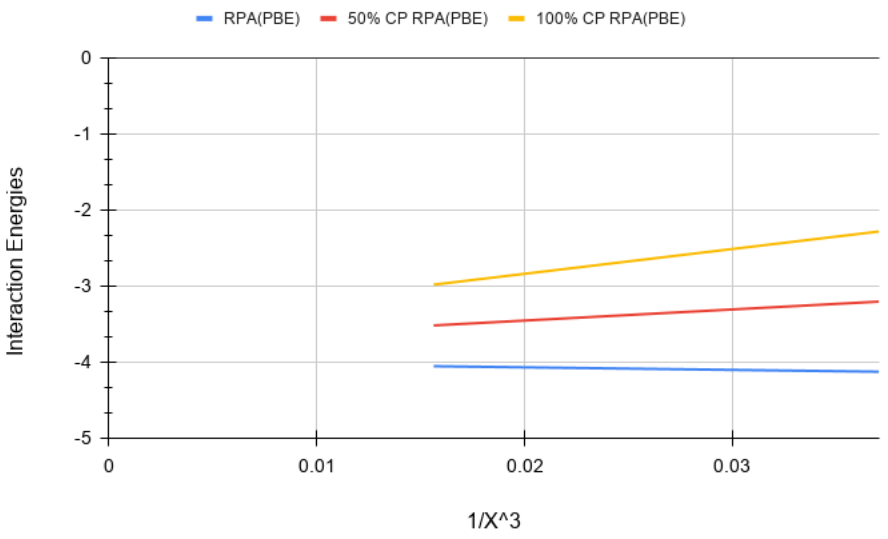



(a) RPA(TPSS)




(b) This is a figure.

Figure 3: Basis sets convergence plot for RPA(TPSS) and RPA(TPSSh) is presented for complex 8.

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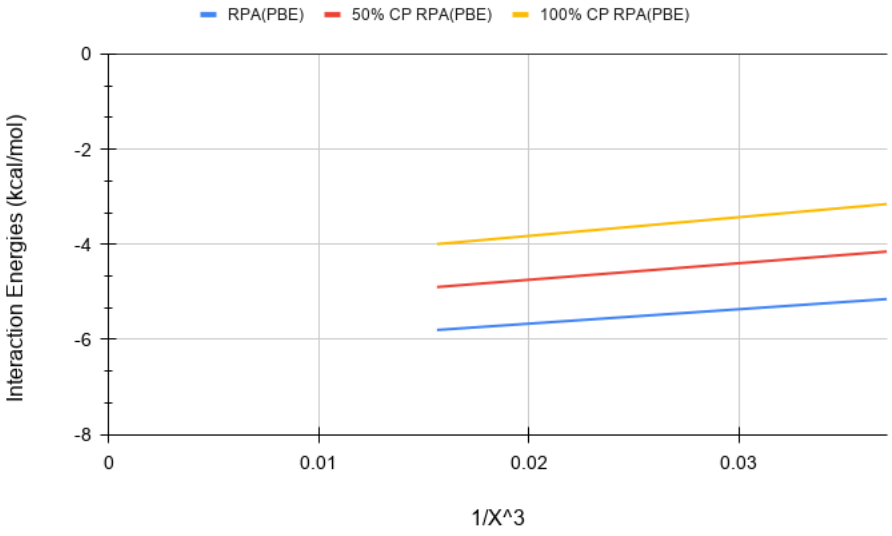


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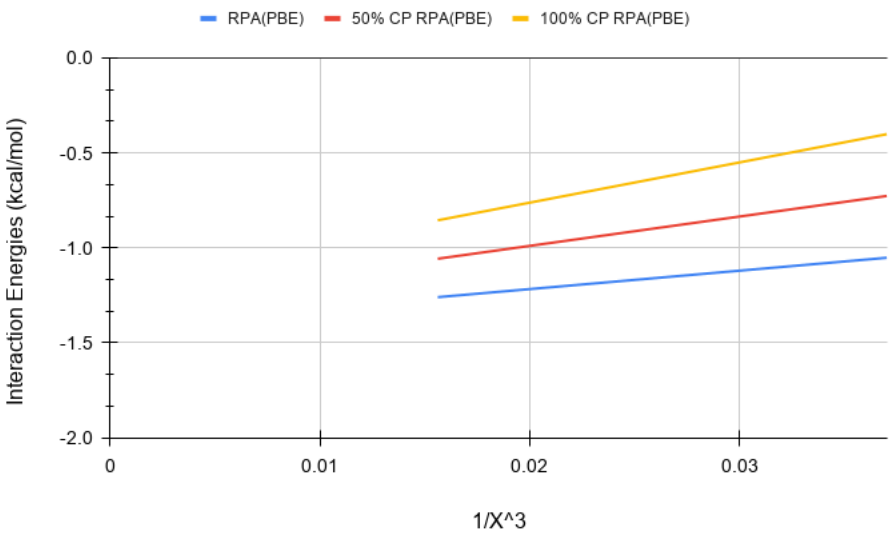


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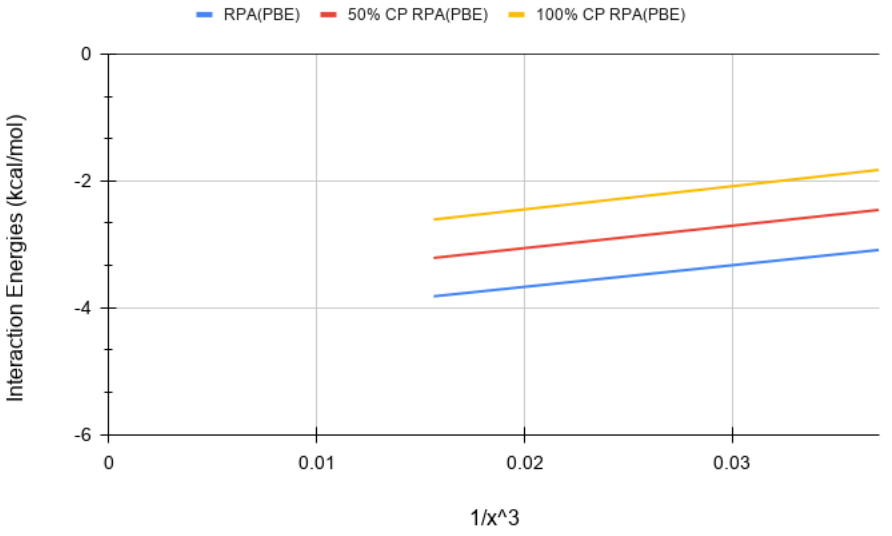


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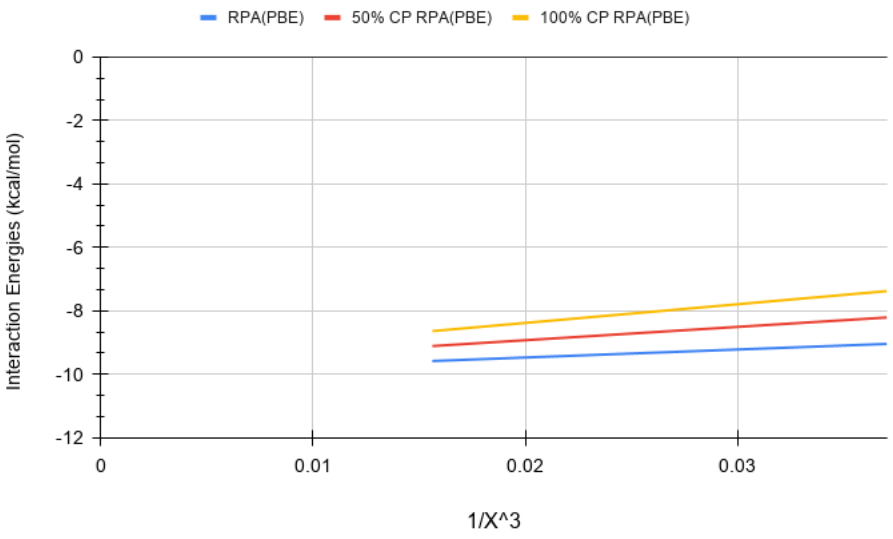


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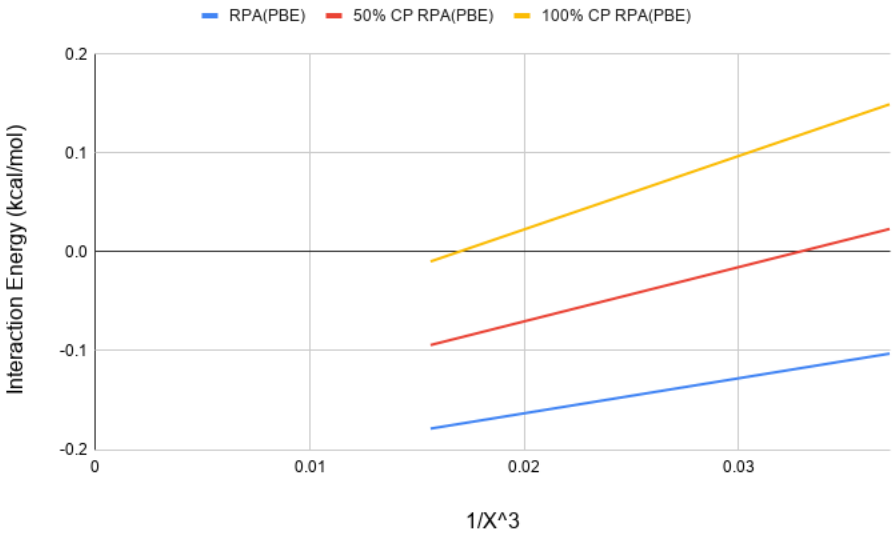


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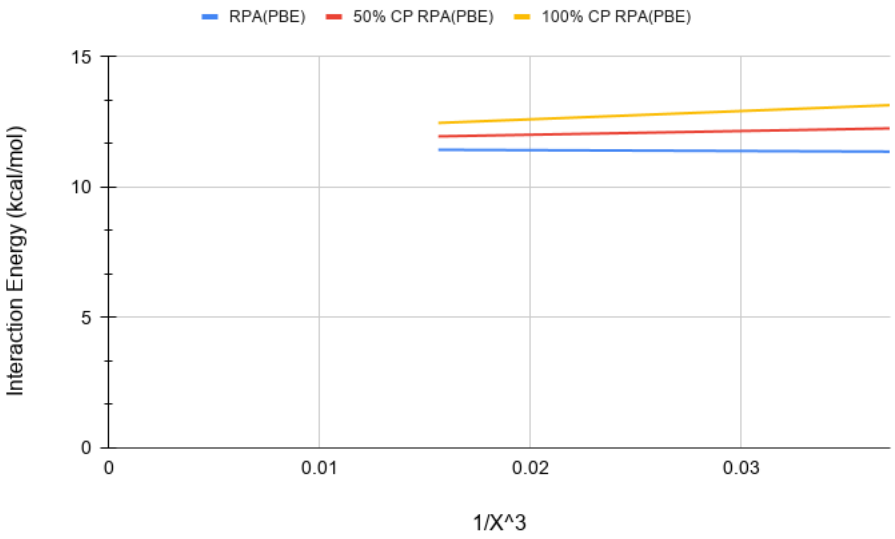


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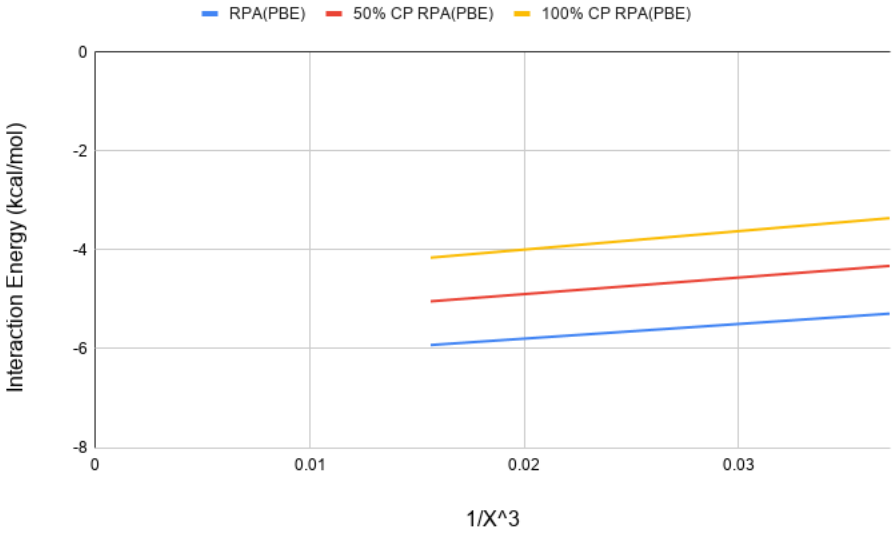


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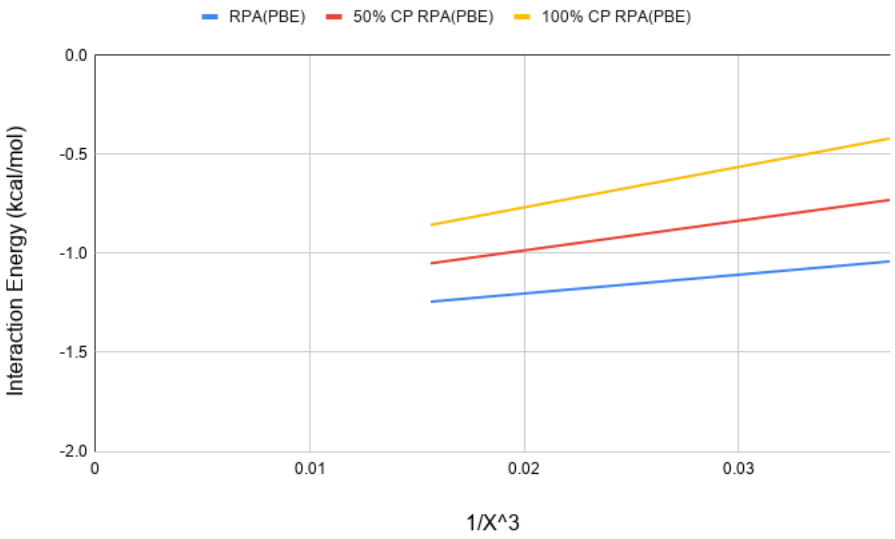


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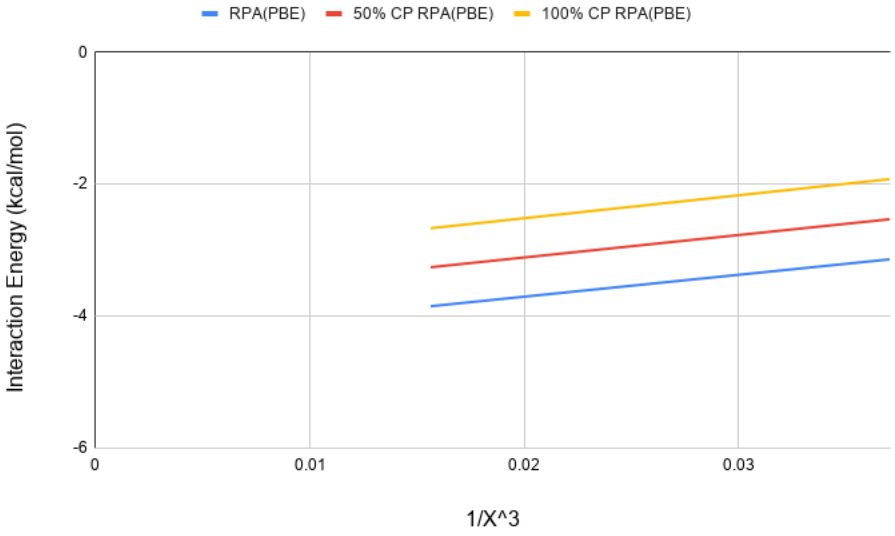


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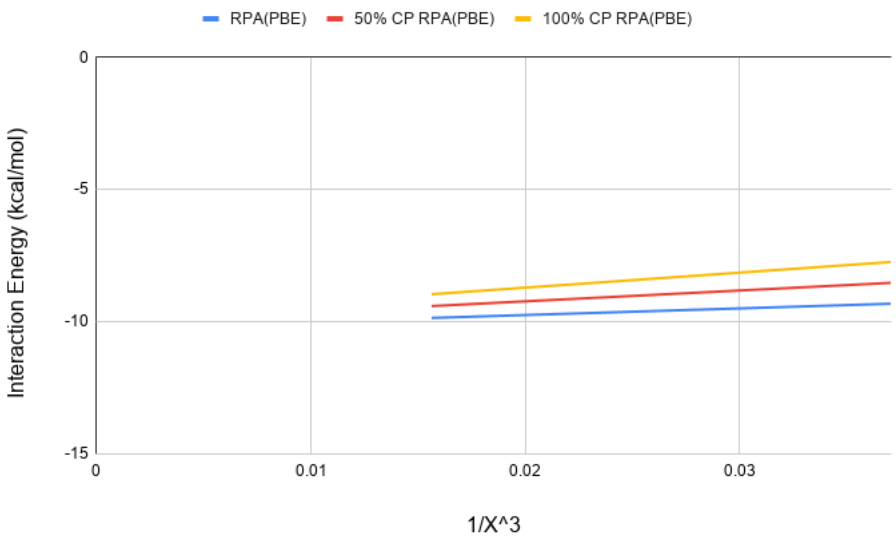


Figure 14: This is a figure.

# 4 Conclusions

This section should answer the following questions: What is the significance of your results for the question, problem, or hypothesis posed in the introduction? What, if any, are the implications in the broader context of the research area laid out in the second paragraph of the introduction?

A second paragraph should discuss any conclusions for your future work. Is there a need to change your approach or your priorities? What remains to be done to reach the goals stated in the first section?