

Dear C. David Sherrill
Associate Editor
Journal of Chemical Physics

Thank you for considering our manuscript for publication in JCP. We have revised the manuscript and hereby resubmit it for your consideration. Below, you find our response to the referee comments and a list of actions taken.

Sincerely yours,
Bjørk Hammer

Reviewer #1 Evaluations:
Recommendation: Publish as is

Thank you for this assessment.
No action taken.

Reviewer #2 Evaluations:
Recommendation: Optional revision
[..]

The manuscript describes advances in the methodology to efficiently search for atomic structures. This is an important problem that currently is receiving considerable attention. The manuscript is clearly written and can be published after the Authors have considered the following minor points:

1) It would be interesting to know how the number of clusters are chosen. Was the number of 5 chosen or was it determined by an algorithm?

The optimal number of clusters was found by the BHO algorithm mentioned in the 2nd last section.
We have inserted a forward reference to that on 3.

2) One could envision problems in determine clusters. Did the Authors encounter any such problems?
We did not encounter any problems. As we use the cluster regularization in a stochastic search any poor clusters would just lead to a single wasted search attempt.

No specific action. We have however inserted a comment on page 6: "The cluster centers found in step 3 will vary depending on the parents and the initialization of the k-means search" that highlights the stochastic nature of the k-means method, which is favorable in the present context.

3) It would be interesting if the clusters could be mapped out in Figure 3.

Yes, but it conflicts somewhat with the flow in our manuscript, since clustering has not been introduced at the time Figure 3 is discussed.

We have inserted the cluster centers used in Figure 4 in the caption for figure 4.

4) For completeness it could be good to report the k-point sampling the electronic structure calculations.

Done on page 2.

5) There are two typos:

Page 3, right column: is-> in

Page 7, left column: og-> of

Corrected. Thank you.