*Editor’s review:*

*You might note that eqn 5 does not match the experimental data for the one electron atomic ions because the Z^4 relativistic correction swamps this effect. The non-adiabatic effect is roughly linear in Z because M is almost linear in Z, 1-mu = 1/(M+1)~ 1/Z.*

We have added a sentence in the manuscript stating this fact.

*There is more interest in the change in the correction with R for diatomics. For H2 we know this is small compared to the actual correction.*

It is indeed possible to calculate R, which we assume to be the inter-nuclei distance for the diatomics, from our wave functions. However, we did not collect that data during our previous calculation. To obtain this data, we would have to rerun all the nonadiabatic DMC calculations, which are the most resource intensive calculations in this project. We would like to have this data as well, but considering the resource and time constraints, it may be better left as future work.

*From your data you could estimate the contribution to the dissociation energy using the non-adiabatic correction your diatomic and atomic energies.*

We have calculated the nonadiabatic correction to the disassociation energies and included them in Table IV.

*You could also estimate the correction to the vibrational frequency.*

Since we treat the entire molecule quantum mechanically, with the electrons and nuclei on the same footing, the ground-state energies that we obtain include energetic contributions arising from ionic vibration as well as nuclear-electron correlation. It is thus unclear how to assign the difference between the nonadiabatic ground-state energy and adiabatic ground-state energy (including ZPE) to the nonadiabatic correction to ZPE versus the nonadiabatic coupling. We may be able to estimate such a correction from the reduced density matrix for the ions, however, this data is not available.

*Reviewer 1:*

*This paper reports the first non-adiabatic Quantum Monte Carlo benchmarks for first row atoms and hydrides, as measured by the diagonal Born-Oppenheimer correction (DBOC) plus the contributions from excited eigenstates. As noted in the text, the DBOC is by far the larger component. Most of the work focuses on total energies for atoms and atomic ions, which are normally not of particular interest to chemists. Beginning on page 6 (out of 8.5 pages of text) the discussion turns to hydrides. Agreement with reference values taken from the literature is good (< 1 mEh) with the exception of HF where the difference grows to 2.4 mEh. In the case of CH the authors believe they have an unusually large fixed-node error.*

*On page 6 the text states, “…the nonadiabatic results agree closely with their adiabatic counterparts…”. That is as expected, but because the dissociation energies in Table II are given as De and then later as D0 it is not possible to tell exactly how large the nonadiabatic corrects actually are. They are quite small. In addition, the DBOCs are relatively insensitive to the level of theory. Perhaps a comment to that effect would be helpful for the reader to put things into perspective.*

*The lack of line numbers in the manuscript makes it difficult to indicate where changes or questions are located in the text.*

*I find the paper to be acceptable for publication after addressing the small number of minor issues below. Minor comments and/or suggests are as follows:*

*Pg. 2 The abbreviation ECG appears to be undefined at this point in the text. Please define. I assume it means “explicitly correlated Gaussian”.*

(explicitly correlated Gaussian) has been added after ECG.

*Pg. 4 Sometimes the term “non-adiabatic” appears in the text and other times it uses “nonadiabatic”. Please be consistent.*

All occurrences of “non-adiabatic” have been replaced with “nonadiabatic”.

*Pg. 6 “Finding accurate reference data…is not straightforward. We will use highly converged ECG data when available.” Break the sentence for the sake of improving the readability.*

This sentence has been broken in half.

*Pg. 7 In the title to Table II it should be made clear that both the total energies and dissociation energies are given in Hartrees. It’s relatively unconventional to report De values in Hartrees.*

We now explicitly state in the caption of Table II that “Both total energies and dissociation energies are given in units of Hartree”.

*Pg. 9 An extraneous lower case “p’ appears in reference 57.*

The typo in the reference has been corrected.

*Reviewer 2:*

*This is a careful study of the handling of non-Born-Oppenheimer electron-nuclear interactions within the realm of Monte Carlo simulations.*