

## Referee 1:

The authors thank the referee for the suggestions and corrections provided.

1. I am not an expert on collision theory, but surely there exist other published calculations of proton-impact cross-sections for H, Li, C, N, Ne, Ar, and small molecules. If so, they should be reviewed in the introduction. If not, that fact should be stated clearly. The paper should not give the impression that these are the first ever ab initio calculations of proton-impact cross-sections.  
On page 10, the authors state "Many ab initio and semi-empirical theoretical approximations have been developed to this end over the last century". This statement should be supported with a few citations.

The references regarding published calculations of inelastic processes and electronic structure methods were included as per suggestion.

2. It should be explained why the T-matrix of Eq. (12) involves orbitals rather than N-electron wave-functions. Is this an approximation? If so, what is its justification?  
The T-matrix of Eq. (12) involves orbitals rather than N-electron wave-functions because the one-electron approximation is being implemented. The approximations employed in our calculations are now clearly stated in the Section 1.

3. Which Ar pseudopotential is shown in Fig. 1? A label is missing.

The Ar pseudopotential is from PARSEC. We include the source in the figure label. The dot-dash line label is missing (corresponding to  $-1/r$ ), but we are now making reference to it in the text.

4. Axis labels in similar figures are not very consistent.

Why does Fig. 6 show differential cross-sections whereas Fig. 8-9 show simply cross-sections?

Why is the horizontal axis in Figs. 5 and 7 labeled "Proton Velocity" whereas in Figs. 6 (for another proton collision) it says "Energy"?

Shouldn't the horizontal axis labels in Figs. 8, 9, 13 say "Photon Energy" rather than simply "Energy"?

The inconsistency of the axis labels in the figures has been fixed. Fig. 6 shows single-differential cross section in order to inspect the scattering of the ionized electron. By computing  $d\sigma/d\varepsilon_f$  we are able to inspect the behaviour of the form factor, which depends of the momentum transfer vector. In Fig. 6, the  $x$  axis corresponds to the scattered electron energy and not incident proton velocity, which is fixed to 1 a.u.). We clarified this in the figure and the text. The "Photon Energy" label was modified in the corresponding Figs.

5. On page 11, the authors state "we considered the methane molecule, which has a suitable spherical geometry". It is a bad choice of words to call the geometry of CH<sub>4</sub> "spherical".

The referee is right, we rephased this sentence properly.

6. Did the basis set used for molecular calculations in Sec. 4.2 (UGBS) include polarization functions? The UGBS as originally defined has no polarization functions and hence is unsuitable for calculations on molecules.

Once again, the referee is correct. The molecular calculations with UGBS should include polarization functions (at least  $d$ -functions) as per shown by Refs. [32,33]. However, to solely isolate the effects of the basis set, we computed the atomic oscillation profiles and the molecular orbitals on the same footing. The results obtained without higher angular momenta than  $L = 1$  should be

approximated. Regardless, when the potential is being optimized, we can minimize to the mean values of our choosing.

7. The analytic form of the second term of Eq. (31) should be justified.
8. Problems with Figs. 1-3 and 5-8: the line samples in the legends are too short to distinguish between solid and dashed lines. The samples should be at least 2.5 times longer. Also, instead of two dashed curves in the plots, one curve should be dashed and the other dot-and-dash to make it possible to distinguish the curves when printed on a b/w printer.

The legend line length and line type have been modified as suggested.

9. Misprints.

Misprints corrected.

10. On page 10, the wording "do to their generally multicentered and highly non-central nature" is awkward. Suggest "due to their nonspherical symmetry and multicenter character".

We thank the referee her/his suggestion and modified it accordingly.

11. Do not capitalize "depurated inversion method" when it is not abbreviated.

The capitalization has been corrected.

12. The references should be formatted in the ACS style, as per AQC instructions.

All references are now formatted in the ACS style.