

## Referee 2:

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

1. The authors develop a simple pseudo-potential (PP) approach to complicated processes of electron capture and transfer and collisions. They show the best results for inverting a many-electron potential to yield effective one-electron charges is by the Depurated Inversion Method they previously published.

We developed an effective potential approach. The inelastic cross sections obtained with it describing the target were compared two different pseudopotentials.

2. The description of numerical difficulties in obtaining the pseudo-charges is detailed, in particular for the 2s AO of the lithium atom. One problem is that a singularity appears due to charge repulsion at around  $r=1$  au. This resembles an electron-electron cusp and could be interpreted physically, because the charges have been defined (although an orbital may be empty) and could be averted by explicit correlation factors.

The referee is correct.

3. Let me comment the CH<sub>4</sub> application.

This uses PPs to replace node-less AOs so it is not a case where the arguments developed and illustrated by fid 1 and 2 are actually applied.

*No entiendo lo que quiere decir. Supongo que cuando dice PP se refiere al DIM? (?)*

4. In below (3), the claim concerning H-atoms is correct but a physical interpretation of the PP in this case is missing.
5. So, for CH<sub>4</sub> oscillations in the AO basis are not modified by use of a PP. They come from defects in the GTO basis as the authors mention.

We did not make use of PPs in the CH<sub>4</sub> calculation.

6. A-why not use an ETO basis? The first term of eq (31) is like an LCAO of Is ETOs. The  $n=2$  shell could be compared with simple semi-cartesian Sturmians:

$$S(1) = N (s+x+y+z) A(r)$$

$$S(2) = N (s-x-y+z) A(r)$$

$$S(3) = N (s-x+y-z) A(r)$$

$$S(4) = N (s+x-y-z) A(r)$$

Here  $N=1/2$  for orthonormal functions,  $A(r) = \exp(-(Z_{eff} r)/2)$   $s = (2/a - r)$  and  $x, y, z$  are just the Cartesian functions. They are bases for the Irreps  $a_2$  ( $S(1)$ ) and  $t_1$  ( $S(2), S(3), S(4)$ )  $Z_{eff}$  is to be optimised and could be given a value from the Clementi tables.

Actually, in our first calculation for a CH<sub>4</sub> potential, we employed the SCF OCE MOs given by Moccia (1964), which uses Slaters. The MOs showed incorrect cusp behaviour and were not considered. However, it is worth inspecting the viability of using CETO.

7. It is well-known that modest GTO basis sets introduce oscillations, since  $\text{grad}[\rho]/\rho$  is not smooth.

This assertion is correct.

8. The FD finite difference HF seems to cure this and it should be benchmarked against ETOs.

9. I would suggest that NaH would be a nice example, with a 10-electron core PP and comparison to the detailed study of Li and H.

This molecule suggestion will be taken into account for further calculations.

10. However, the desired properties are obtained quite well.

A small point is that a PP is not the same as GGA which is a family of functionals. The ABINIT GGA is PBE by default and the PP is calculated within that framework. The important point is that it is norm-conserving.

The referee is right.

11. The English is rather poor.

Misprints have been corrected, and awkward sentences have been rephrased.