Referee 2:

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

1. `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.

2. `Let me comment the CH4 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.`

   `In below (3), the claim concerning H-atoms is correct but a physical interpretation of the PP in this case is missing.`

   H has only one electron, and it does not seem to have any use to calculate the corresponding pseudopotential. However, there are many different proposals for PP, reproducing with high accuracy the main features of the wavefunctions, even for excited states.

3. `So, for CH4 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 CH4 calculation.

4. `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 othonormal 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 a2 (S(1)) and t1 (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 CH4 potential, we employed the SCF OCE MOs given by Moccia (1964), which uses Slaters. The inversion of such MOs showed incorrect behaviour of the charge in the origin and, therefore, they were not considered. However, it is worth inspecting the viability of employing ETOs in further calculations.

5. `It is well-known that modest GTO basis sets introduce oscillations, since grad[`ρ`]/`ρ` is not smooth.`

   This assertion is correct and it is clearly demonstrated in Ref. [28].

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

   Yes, the FD method cure the oscillation issue, however, the poles due to the nodes and asympotic divergences will still be present.

7. `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.

8. `However, the desired properties are obtained quite well.`

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   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 it that it is norm-conserving.
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   The referee is right.

9. `The English is rather poor.`

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