Yannick Carissan
Aix-Marseille Université
ISM2, UMR-CNRS-7313
Campus St. Jérôme service 561
F-13397 Marseille cedex 20
France
E-mail Yannick.Carissan@univ-amu.fr
Tel (33) +4.91.28.91.68
Fax (33) +4.91.28.91.79

October 24, 2018

Dear editor,

This is the second submission of this article entitled **"Atomic pseudo-potentials for reproducing the valence electron behaviour of $sp^2$ carbon atoms "** in which we present new pseudo-potentials to be used for $sp^2$ carbon atoms. It was not accepted for publication in the Journal of Computational Chemistry but we would like to be given a second chance for publication in this journal as we strongly believe that it is a work relevant to this journal. We have worked on improving the manuscript over the last year. We have taken into account all remarks made by the referees, improved the presentation and the discussion to clarify some important points, added new results and an analysis of our results by use of a topological analysis of the density (AIM).

In this work, we aim at reproducing the anisotropy of the hybridised carbon atom by employing semi-local atomic pseudo-potentials as already implemented in most quantum chemistry program packages. Thus, no programming from the user is required. Only the parameters we extract and publish in this work are needed to reproduce these potentials for any molecule with such carbons. These pseudo-potentials for recreating $sp^2$ carbon atoms are built and tested as a building block for various all-trans-polyenes and polycyclic aromatic hydrocarbons. The pseudo-carbon we develop has a nuclear charge of 1, thus only one electron is treated explicitly. It is employed in ab-initio calculations in which several physical characteristics including 1st ionisation and excitation energies, as well as the HOMO energy, are found to be well-reproduced by the pseudo-system. Furthermore and newly, we show in this work that highly excited states (20 singlets and 20 triplets using TD-DFT) can be reproduced with our method at low computational cost. Finally an AIM study shows that the $\pi$ density is very similar to the $\pi$ density of all-electron calculations.

To the best of our knowledge, this is the first time such a potential, localised fully to the atom which it replaces, has been developed.

We think, this work is in line with aims and scope of the Journal of Computational Chemistry.

The authors are :

- Alexander Punter
- Dr. Paola Nava
- Dr. Yannick Carissan, corresponding author (see address in the header)

With our Best Regards,

Yannick Carissan