Dr. 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

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Dear editor,

In the submitted article, entitled **"sAtomic pseudo-potentials for reproducing the valence electron behaviour of sp2 carbon atoms "**, we present new pseudo-potentials to be used for sp^2 carbon atoms. Our strategy consists in reproducing the anisotropy of 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 hydrocarbon chain and ring systems. This pseudo-system 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.
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 Computational and Theoretical Chemistry.

The authors are :

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

We suggested a set of 3 reviewers, with no preference. According to us, the three of them are relevant to review this paper.

With our Best Regards,

Dr. Yannick Carissan