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Dear editor,

This article entitled **"Atomic pseudo-potentials for reproducing the valence electron behaviour of sp^2carbon atoms"** was transferred to you from our submission to the Journal of Computational Chemistry. In this work, we present new pseudo-potentials to be used for sp^2 carbon atoms. 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, 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 π density is very similar to the π 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 International Journal of Quantum 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