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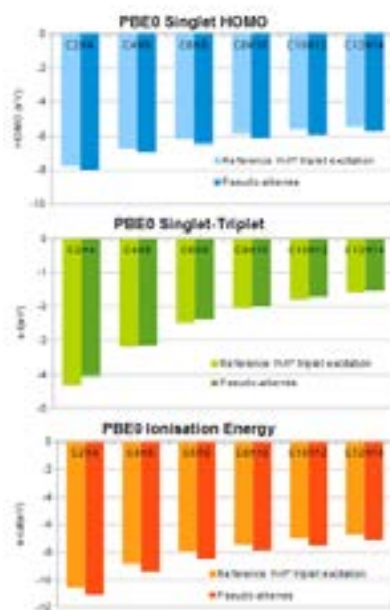
# PHYSICAL AND THEORETICAL CHEMISTRY

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## An embedding technique based on a strategic use of atomic pseudo potentials

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Atomic pseudo potentials were primarily used to replace core electrons in quantum chemistry calculations. Since 2013, we decided to use pseudo potentials to model core and valence electrons for hybridized atoms. In this work, we focus on the  $sp^2$  carbon atom. We decided to begin with a pseudo-carbon, and used the  $CH_3$  radical as a reference to which we tried to optimize the model. Starting with a pseudo-carbon with a charge of one, and one electron, we were able to use potentials to force the occupation of specific orbitals, and to manipulate the energy levels of these orbitals. In practice, the only way to make the s potentials affect the orbitals was not to place them on the molecular plane itself, thus we ended up with a scheme that had potentials above and below the plane. After confirming the model worked on the ethene molecule, we were able to reproduce good accuracy characteristics such as ionisation and excitation energies across a range of molecules including chain alkenes and aromatic, cyclic compounds. Unlike in previous attempts, we are now able to extract atom based pseudo potentials: no bond centered potential is now required making the scope of use of these potentials extremely large. In order to be useful, these potentials must be able to replicate their results across other systems. Testing them with some of the systems used in Carissan & Drujon, we have met with success. A single set of optimized potentials give results within  $\sim 0.5$  eV of reference calculations over HF, DFT and TD-DFT calculations.



## Biography

Yannick Carissan is an Assistant Professor at Aix-Marseille University. He is an expert in Theoretical Chemistry and focuses on the interaction between research and teaching. His model based on chemically relevant concepts is an attempt to fill the gap between empirical methods and *ab initio* full electron quantum chemistry calculations.

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