Pseudopotential-Fragment Spectroscopy for Organic Molecules and Carbon Allotropes

Alexander Punter[1], Paola Nava[2], and Yannick Carissan[3]

[1]Université d'Aix-Marseille
[2]Aix-Marseille Université
[3]Institut des Sciences Moleculaires de Marseille

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Abstract

Building on a previous work, pseudopotential sets are developed and tested for a variety of sp^2 and sp^3 carbon fragments. These fragments contain only one or two explicit protons and electrons, and make use of non-atom-centred potentials. They are tested with Density Functional Theory calculations in a selection of chemical environments in which several physical characteristics, including orbital and first ionisation energies, are found to be well-reproduced. They are then employed in the reproduction of molecular absorption spectra for large organic molecules and carbon allotropes, and are found to recreate both absorption and ECD spectra to a high accuracy. They are also found significantly to increase the computational efficiency of TDDFT calculations in which they are used.

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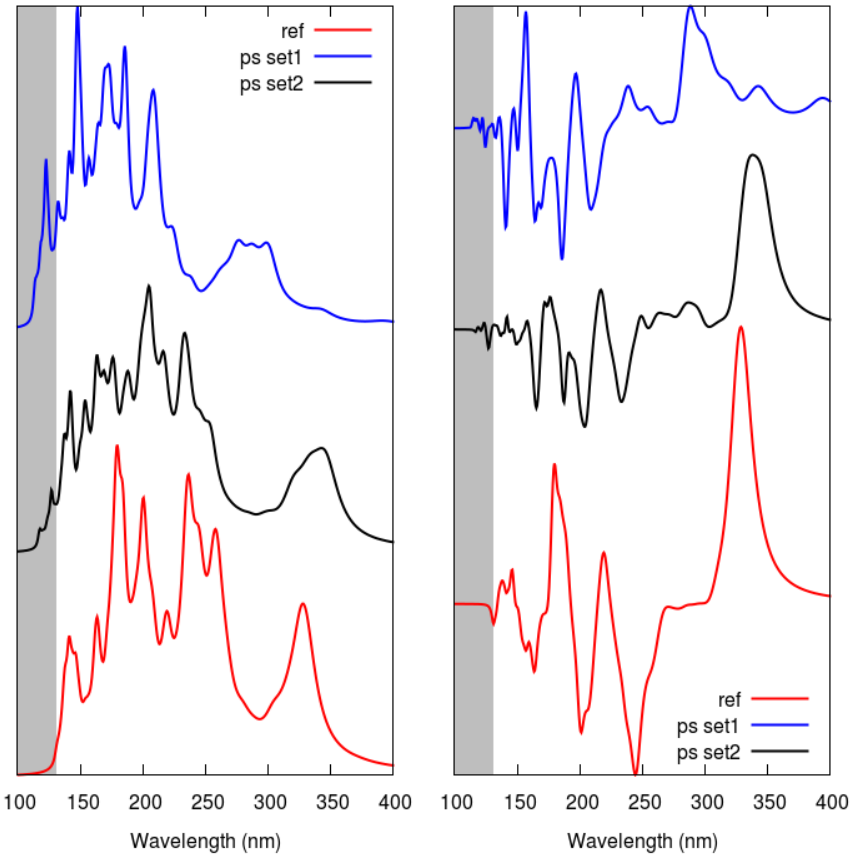

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