Overview of selected configuration interaction and its coupling with DFT

Emmanuel Giner*[1]

[1]Laboratoire de Chimie Théorique – CNRS : UMR7616 – France

Résumé

The purpose of this talk is to give a brief (and non exhaustive) introduction and overview of the concept of selected CI and its application in modern quantum chemistry. More specifically, I will present the algorithm available in the open-source software Quantum Package and show some of the applications already performed.
Eventually, I will discuss about the basis set which consists in one of the major the limitations of wave function theory, and briefly introduce a very recently introduced approach based on DFT aiming at curing this problem.

Mots-Clés: wave function, DFT, selected CI

*Intervenant