Overview of selected configuration interaction and its coupling with DFT

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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[1] 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[2].

References
