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

[1] Y. Garniron, K. Gasperich, T. Applencourt, A. Benali, A. Ferté, J. Paquier, B. Pradines, R. Assaraf, P. Reinhardt, J. Toulouse, P. Barbaresco, N. Renon, G. David, J. P. Malrieu, M. Véril, M. Caffarel, P. F. Loos, E. Giner, and A. Scemama. Quantum package 2.0: A open-source determinant-driven suite of programs. *J. Chem. Theory Comput.*, 15:3591, 2019.

[2] E. Giner, B. Pradines, A. Ferté, R. Assaraf, A. Savin, and J. Toulouse. Curing basis-set convergence of wave-function theory using density-functional theory: A systematically improvable approach. *J. Chem. Phys.*, 149:194301, 2018.