Many-body Green's function and state-specific CI methods for excited states

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In this talk, I will present some of our recent advances on many-body Green's function methods and their connections to coupled-cluster (CC) theory [1]. In particular, I will show how to recast the *GW* and Bethe-Salpeter equation (BSE) as non-linear CC-like equations. Similitudes between BSE@*GW* and the similarity-transformed equation-of-motion CC method introduced by Nooijen will be also put forward. I will also introduce a new systematically improvable route for excited-state calculations, state-specific configuration interaction (ΔCI), in which, starting with a reference built from optimized configuration state functions, separate CI calculations are performed for each targeted state [2]. Accounting for single and double excitations produces the ΔCISD model, which can be improved with second-order Epstein-Nesbet perturbation theory (ΔCISD+EN2) or a posteriori Davidson corrections (ΔCISD+Q). These models will be gauged against a vast and diverse set of 294 reference excitation energies [3].

[1] R. Quintero-Monsebaiz, E. Monino, A. Marie, and P. F. Loos, *J. Chem. Phys.* **157**, 231102 (2022).

[2] F. Kossoski and P. F. Loos, *J. Chem. Theory Comput.* (submitted) arXiv:2211.03048.

[3] M. Véril, A. Scemama, M. Caffarel, F. Lipparini, M. Boggio-Pasqua, D. Jacquemin, and P. F. Loos, *WIREs Comput. Mol. Sci.* **11**, e1517 (2021).