Ensemble density functional theory of electronic excitations: Key features of the exact theory, extensions, and practical approximations

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In the first part of the presentation I will revisit the concept of exchange-correlation derivative discontinuity within the ensemble density functional theory (eDFT) of neutral electronic excitations [1,2]. For that purpose, I will introduce the so-called extended *N*-centered eDFT formalism [3,4] where the Theophilou-Gross-Oliveira-Kohn (TGOK) ensemble description of neutral excited states [5-7] is combined with an *N*-centered ensemble description of ionization processes [8-10]. In a second part, I will discuss the extension of eDFT to the time-dependent linear response regime [11] and how it could be used in the design of ensemble density-functional approximations. If time permits, I will also discuss the use of eDFT (or alternative density-functional approaches) in the beyond-Born-Oppenheimer description of molecular systems [12].

References

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