

Stochastic Time-Dependent Current-DFT: a functional theory of open quantum systems

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”Standard” density-functional methods can only deal with Hamiltonian dynamics, and not with open quantum systems, namely systems dynamically coupled to baths/reservoirs. There is, however, a large class of physics problems where one needs to consider this interaction explicitly. These include energy relaxation and dephasing, non-radiative decay, quantum measurement theory, etc. In order to address these issues, we have introduced a new theory we have named Stochastic TD-CDFT [1,2] and extended it to the correlated motion of electrons and ions [3]. I will describe this theory in detail, its range of applicability, and show some applications with and without ionic motion.

[1] M. Di Ventra and R. D’Agosta, *Stochastic Time-Dependent Current-Density-Functional Theory*, Phys. Rev. Lett. **98**, 226403 (2007).

[2] R. D’Agosta and M. Di Ventra, *Stochastic Time-Dependent Current-Density-Functional Theory: a functional theory of open quantum systems*, **78**, 165105 (2008).

[3] H. Appel and M. Di Ventra, *Stochastic Quantum Molecular Dynamics*, Phys. Rev. B **80**, 212303 (2009).