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Time-dependent density functional theory for open quantum systems DAVID TEMPEL, ALAN ASPURU-GUZIK, Harvard University — We present the extension of time-dependent density functional theory (TDDFT) to the realm of open quantum systems (OQS). OQS-TDDFT allows a first principles description of electronic systems undergoing non-unitary dynamics due to coupling with a bath, such as that arising from molecular vibrations, solvent degrees of freedom or photon modes of the electromagnetic field. We first prove extensions of the Runge-Gross and van Leeuwen theorems to OQS-TDDFT, which rigorously establish it as a formally exact theory. We then discuss development of approximate OQS-TDDFT functionals, exact conditions on these functionals, as well as future challenges. Finally, we will discuss the application of OQS-TDDFT in obtaining broadened absorption spectra.

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