

Abstract Submitted
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Revealing Open Quantum Systems with Subsystem DFT ALISA KRISHTAL, MICHELE PAVANELLO, Rutgers University - Newark — The traditional quantum chemical methods, wave function or density based, are designed to solve for a closed system, where the Hamiltonian contains all relevant interactions. The closed system is, however, not realistic, as in real life the system is embedded in an environment with which it interacts to some degree. Including the description of the environment at the full quantum mechanical level leads to the Open Quantum Systems (OQS) theory: the only theory which can describe non-Markovian dynamics between the system and the environment. By allowing the flow of information in both directions phenomena such as quantum entanglement, relevant for the design of quantum computers, become available. While most OQS theories rely on the density matrix to describe the system-bath interaction, time-dependent subsystem DFT[1,2] allows to approach the problem using the electron density. Through Dyson-like equations connecting the density-density response kernels of the OQS and its environment, the extent to which non-Markovian dynamics is present can be revealed. We illustrate this for the process of excitation energy transfer in coupled chromophores embedded in explicit solvent. [1] M. Pavanello, *J. Chem. Phys.* 138, 204118 (2013). [2] A. Krishtal et al. *J. Chem Phys.* 142, 154116 (2015).

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