Revealing Open Quantum Systems with Subsystem DFT ALISA
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tional 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 dynam-
ics between the system and the environment. By allowing the flow of information
in both directions phenomena such as quantum entanglement, relevant for the de-
sign of quantum computers, become available. While most OQS theories rely on
the density matrix to describe the system-bath interaction, time-dependent subsys-
tem 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