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Modelling Charge Transfer Reactions and Excitations with Subsystem DFT[1] MICHELE PAVANELLO, Leiden University, JOHANNES NEUGEBAUER, Technical University Braunschweig — The subsystem formulation of DFT known as Frozen Density Embedding (FDE) offers an excellent platform for studying charge transfer reactions in solvated systems, such as biosystems. We present the necessary theory developments for the calculation of the electronic couplings as well as the charge transfer excitations from FDE derived densities. We present preliminary calculations on DNA oligomers radical cations that include donor-bridge, donor-bridge-acceptor, and fully solvated systems.

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Michele Pavanello
Leiden University

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