Abstract Submitted
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Energy and charge transfer in photoexcited molecules - A challenge for TDDFT[1] ESPEN SAGVOLDEN, FILIPP FURCHE, UC Irvine — We study charge-transfer excitations and radiationless energy transfer between two chromophores (parts of a molecule which are individually excitable). These reactions have widespread chemical significance, particularly to the design of organic solar cell panels and molecular switches and to photosynthesis. Time-Dependent DFT (TDDFT) offers a very favorable relationship between accuracy and calculational cost in many cases. Calculations are performed for the (2-pyridone)$_2$-dimer which is experimentally well-characterized [1]. TDDFT is compared to experiment and competing methods such as Time-Dependent Hartree-Fock, CI singles, and coupled-cluster methods.
[1] A. Müller, F. Talbot, and S. Leutwyler, J. Chem. Phys. **112**, 2836 (2002).

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