CFEL SCIENCE

SEMINAR

09th May 2018 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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Simulation of quantum dynamics and transport using multiconfiguration wave-function methods

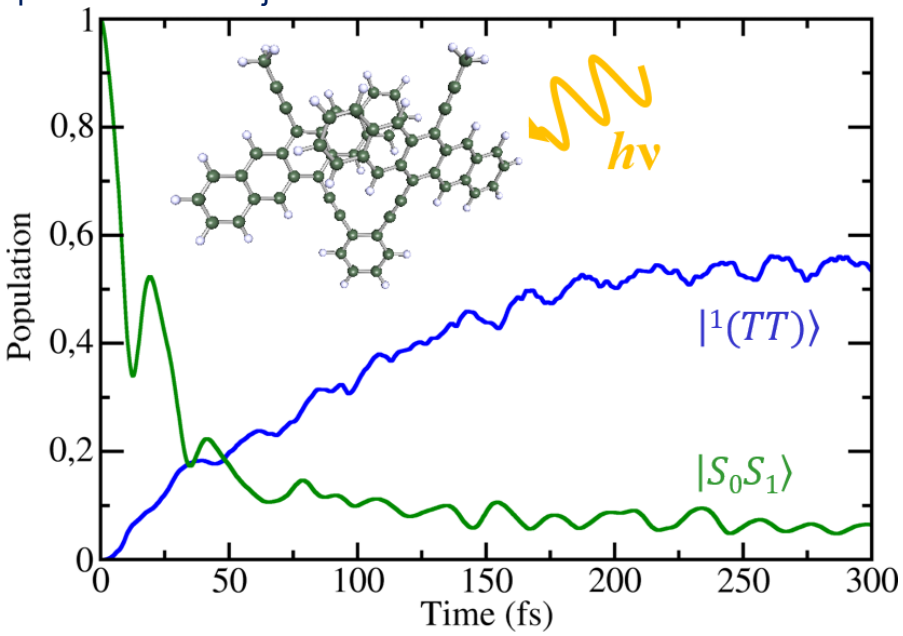
The accurate theoretical treatment and simulation of quantum dynamical processes in many-body systems is a central goal in chemical and condensed matter physics. In this talk, the multilayer multiconfiguration time-dependent Hartree (ML-MCTDH) method [1] is discussed as an example of an approach that allows an accurate description of quantum dynamics and transport in systems with many degrees of freedom. The ML-MCTDH method is a variational basis-set approach, which uses a multiconfiguration expansion of the wave function employing a multilayer representation and time-dependent basis functions. It extends the original MCTDH method [2] to significantly larger and more complex systems. Employing the second quantization representation of Fock space, the ML-MCTDH method can also be used to treat the dynamics of indistinguishable particles [3,4]. Illustrative applications of the methodology to charge and energy transport processes are discussed, including photoinduced electron transfer, intramolecular singlet fission, and electron transport in molecular junctions.

[1] H. Wang and M. Thoss, J. Chem. Phys. 119, 1289 (2003); H. Wang, J. Phys. Chem. A 119, 7951 (2015).

[2] H.-D. Meyer, U. Manthe, and L.S. Cederbaum, Chem. Phys. Lett. 165 , 73 (1990).

[3] H. Wang and M. Thoss, J. Chem. Phys. 131, 024114 (2009); 145, 164105 (2016).

[4] E. Wilner, H. Wang, M. Thoss, E. Rabani, Phys. Rev. B 89, 205129 (2014).



Host: Robin Santra – CFEL-DESY Theory Division