

## The 16th Femtochemistry Conference (FEMTO16)



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# Nonlinear Femtosecond Signals at Finite Temperature including Static Disorder via a Thermo Field Dynamics-Tensor Train Method

*Monday, June 23, 2025 5:00 PM (20 minutes)*

We have developed a fully quantum, numerically accurate wave function-based approach for the calculation of third-order spectroscopic signals of polyatomic molecules and molecular aggregates at finite temperature including static disorder effects. The systems are described by multimode nonadiabatic vibronic-coupling Hamiltonians, in which diagonal terms are treated in harmonic approximation, while off-diagonal interstate couplings are assumed to be coordinate independent. The approach is based on the Thermo Field Dynamics (TFD) representation of quantum mechanics and Tensor-Train (TT) representation of the vibronic wave function, providing a very efficient numerical simulation of quantum evolution of systems with many degrees of freedom. The effect of static disorder is included using a novel approach based on auxiliary harmonic oscillators variables. The developed TFD-TT approach is applied to the calculation of time- and frequency-resolved fluorescence spectra of the Fenna–Matthews–Olson (FMO) antenna complex at room temperature taking into account finite time-frequency resolution in fluorescence detection, orientational averaging, and static disorder.

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