“Simulation of quantum molecular dynamics in the condensed phase: rate constants, correlation functions and nonequilibrium dynamics”

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Quantum dynamical effects play a central role in a variety of important processes that take place in condensed-phase environments. Important examples, which are particularly relevant for chemistry, include proton and electron transfer reactions, vibrational relaxation, chromophore spectroscopy and photochemistry. At the same time, a numerically exact solution of the Schrodinger equation in the case of many-body systems remains far beyond the reach of currently available computer resources, due to the exponential scaling of the computational effort with the number of degrees of freedom. I will report on recent progress that was made in my group toward developing and employing different types of approximate methods for computing experimentally relevant quantities, such as rate constants and response functions, in such systems. I will also present a new approach for simulating non-equilibrium quantum dynamics, which is based on calculating the memory kernel of the generalized quantum master equation for an arbitrary system-bath coupling.