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**Calculation of Dissipation Pathways in Quantum Chemical Dynamics**

Quantum chemical dynamics in condensed phase often involves a macroscopic number of degrees of freedom (DOF), and is often treated under the framework of open quantum systems. For this purpose, over the past few decades, a number of theoretical methods have been developed to study how the central DOFs evolve over time. However, studying fundamental principles underlying the dynamics often requires locating the surrounding DOFs that play major roles in the process, which often cannot be readily achieved based on conventional simulation methods. In this presentation, we suggest that this theoretical challenge can be overcome by focusing on time-dependent dissipation between the subsystem and surroundings, which encodes the progress of energy relaxation occurring along the dynamics. We will introduce our recently constructed theoretical framework which enables efficient decomposition of dissipation into contributions from individual surrounding DOFs, based on quantum master equation derived under projection operator technique. The developed method is benchmarked against numerically exact simulation method and then applied to a realistic model of a light-harvesting protein complex to demonstrate its usefulness.

**References**

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