

Exploring Quantum Dynamics: From Molecular Complexity to Computational Models

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The microscopic quantum world is increasingly present in our everyday lives and technology. To keep up, we need to advance theoretical and numerical tools capable of handling highly dimensional, coupled, and correlated quantum systems. For molecules, this task is especially challenging due to strong, anharmonic interactions among nuclei and electrons.

In this talk, I will discuss state-of-the-art numerical methods based on tensor decomposition used to describe high-dimensional quantum dynamics in molecules and other complex systems. I will then examine two recent, distinct applications of these tools: first, in analyzing the dynamics and quasi-thermalization of excited molecular clusters, and second, in studying how vibrational-electronic coupling influences long-range transport in exciton-polaritons.