

## The Department of Chemistry Presents:

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"Light Matters: Quantum Control of Molecules through Light-Matter Coupling"

Light-matter interactions dictate phenomena from color perception and vision to photosynthesis, solar energy conversion, and spectroscopic analysis. Advances in ultrafast spectroscopy and quantum simulation now allow us to probe and influence these interactions at the natural timescale of the electron, enabling the quantum control of chemical dynamics and reactivity. In this lecture, I will highlight recent developments in ab initio real-time electronic structure methods for describing ultrafast light-matter interactions. Illustrative examples include controlling intersystem crossing in transition-metal complexes and modulating dipole-switching dynamics in molecules coupled to optical cavities. These methods, together with the software tools required for their implementation, open new opportunities for controlling chemical processes, advancing quantum technologies, and designing bespoke functional materials. I will conclude with the proposed extension of these methodologies to new frontiers, namely, the incorporation of Floquet theory and machine-learning algorithms for reduced computational scaling. Together, these theoretical advances are poised to deepen our fundamental understanding and expand the practical quantum control of time-dependent molecular phenomena.

Monday, December 15, 2025 @ 4 P.M. 1220 Chemistry Building