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Controlling nuclear quantum dynamics with shaped laser pulses

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The use of tailored laser pulses to control chemical processes has received much attention over the last 25 years, in part due to the rapid development of experimental pulse shaping techniques. This has permitted studies of control in an ever widening array of systems with increasing complexity (i.e., dimensionality for molecules). In this talk, I will present our computational approach for these problems involving the use of optimal control theory (OCT) for determining laser pulse shapes combined with the multi-configurational time-dependent Hartree (MCTDH) approach for solving the quantum dynamics. MCTDH is a useful approach for solving high-dimensional (4D-21D) problems for molecules. However, for efficiency, MCTDH requires the underlying molecular potential energy and dipole moment surfaces in product form. I will present recent efforts to determine potential energy surfaces for HFCO and HONO based on high-level ab initio results. If time permits, I will discuss initial efforts on the control of dynamics in these systems.

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