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Title: Nuclear-Electronic Orbital Approach for Electronic, Vibrational, and Vibronic Polaritons

Abstract: The nuclear-electronic orbital (NEO) method treats electrons and specified nuclei quantum mechanically on the same level, inherently capturing nuclear quantum effects such as nuclear delocalization, zero-point energy, and tunneling, as well as non-Born—Oppenheimer effects. Real-time NEO simulations numerically integrate the time-dependent Schrödinger for both electrons and specified quantized nuclei to calculate spectra and simulate ultrafast dynamics. Coupling these simulations to a photonic cavity mode provides a versatile platform in which both electronic and vibrational strong coupling can be studied at the same level of theory. In this talk, I will present results displaying nuclear-electronic quantum dynamics when coupled to a cavity mode, including excited state intramolecular proton transfer, light-matter entanglement, vibronic strong coupling, and hydrogen tunneling.