**Integrating Electronic and Nuclear Quantum Effects**

**in Quantum Chemistry and Dynamics**

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Nuclear quantum effects such as zero-point energy, nuclear delocalization, and tunneling play an important role in a wide range of chemical and biological processes. The nuclear-electronic orbital (NEO) approach incorporates nuclear quantum effects and non-Born-Oppenheimer effects into quantum chemistry calculations and molecular dynamics simulations. This approach treats specified nuclei, typically protons, quantum mechanically on the same level as the electrons with multicomponent density functional theory (DFT) or wave function methods. Nuclear delocalization and anharmonic zero-point energy are inherently included in molecular energy calculations, geometry optimizations, reaction paths, and dynamics. The NEO approach also provides accurate descriptions of excited electronic, vibrational, and vibronic states, as well as nuclear tunneling and nonadiabatic dynamics. The real-time NEO methods enable nonequilibrium nuclear-electronic dynamics simulations beyond the Born-Oppenheimer approximation for the investigation of thermal and photoexcited chemical reactions. These simulations can be performed in implicit or explicit solvent, proteins, or periodic solids. This talk will present foundational and recently developed NEO methods, as well as applications to photoinduced proton transfer, hydrogen tunneling, proton-coupled electron transfer, molecular polaritons, and plasmon-driven processes.