Importance of the quantum-mechanical (QM) effects associated with the nuclei is gaining recognition in chemistry and physics, as researchers manipulate matter, light, electric and magnetic fields at the atomistic level for advanced materials applications. For example, the isotope dependence of the proton conductance in low-dimensional boron nitrides, and of the crystallinity of poly(3-hexylthiophene) [1] is attributed, in part, to the nuclear quantum effects. The development of a general dynamics approach, incorporating the nuclear quantum effects and scalable to large molecular systems, remains an outstanding theoretical challenge because of the exponential scaling of computational costs with the system size. We will describe exact [2] and approximate dynamics, inspired by the quantum trajectory formulation of the Schrödinger equation [3]. The underlying trajectory framework is particularly efficient in describing the large-amplitude nuclear motion and is well suited for a hierarchical [exact QM/approximate QM/classical] treatment of a quantum system coupled to the molecular environment.

References