Commonly-used adiabatic molecular dynamics methods, where dynamical propagation is subject to only one potential energy surface (PES), are not sufficient for studying charge transfer reactions which normally involve participation of several electronic and/or vibrational states plus nuclear quantum effects such as proton tunneling and zero point energy. During the past few years, we have developed different methods and schemes to tackle this challenge with an emphasis on proton-coupled electron transfer (PCET) reactions. (1) We have developed a surface-hopping algorithm based on the solution of the mixed quantum-classical Liouville (MQCL) which compared to the widely-used fewest-switches surface-hopping (FSSH) approach provides a more rigorous treatment of decoherence yielding accurate mechanisms and rate constants for PCET reactions. (2) Further, to efficiently simulate non-adiabatic effects and nuclear quantum effects with large number of degrees of freedom, we developed a Ring Polymer Surface-Hopping (RPSH) method where the nuclei are quantized through ring-polymer Hamiltonian in an extended phase-space. Hence, RPSH incorporates nuclear quantum effects into classical propagation yielding the correct physical behavior of quantum systems where classical FSSH fails. (3) To provide accurate and convenient on-the-fly dynamics propagations, we have recently developed quasi-diabatic (QD) scheme for interfacing exact diabatic quantum dynamics methods with adiabatic electronic structure calculations packages. We demonstrated the applicability and accuracy of this QD scheme in the context of studying non-adiabatic dynamics of both thermally-induced and photo-induced PCET reactions.