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**Nonadiabatic dynamics of photo-induced proton-coupled electron transfer reactions via ring-polymer surface hopping.** FARNAZ SHAKIB, PENGFEI HUO, University of Rochester — Photo-induced proton-coupled electron transfer reactions (PCET) are at the heart of energy conversion reactions in photocatalysis. Here, we apply the recently developed ring-polymer surface-hopping (RPSH) approach to simulate the nonadiabatic dynamics of photo-induced PCET. The RPSH method incorporates ring-polymer (RP) quantization of the proton into the fewest-switches surface-hopping (FSSH) approach. Using two diabatic electronic states, corresponding to the electron donor and acceptor states, we model photo-induced PCET with the proton described by a classical isomorphism RP. From the RPSH method, we obtain numerical results that are comparable to those obtained when the proton is treated quantum mechanically. This accuracy stems from incorporating exact quantum statistics, such as proton tunnelling, into approximate quantum dynamics. Additionally, RPSH offers the numerical accuracy along with the computational efficiency. Namely, compared to the FSSH approach in vibronic representation, there is no need to calculate a massive number of vibronic states explicitly. This approach opens up the possibility to accurately and efficiently simulate photo-induced PCET with multiple transferring protons or electrons.

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