

# **Nonadiabatic dynamics in the long timescale: The next challenge in computational photochemistry**

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Nonadiabatic dynamics simulations in the long timescale (longer than 100,000 integration timesteps) are the next challenge in computational photochemistry.<sup>1</sup> In this talk, we will explore the scope of what we expect from methods to run such simulations: they should work in full nuclear dimensionality, be general enough to tackle any molecule, and not require unrealistic computational resources.

We will examine the main methodological challenges we should venture into to advance the field, including the computational costs of the electronic structure calculations, stability of the integration methods, the accuracy of the nonadiabatic dynamics algorithms, and software optimization.

Based on simulations designed to shed light on these issues, we show how machine learning may be a crucial element for long-timescale dynamics, either as a surrogate for electronic structure calculations or aiding the parameterization of model Hamiltonians. We also show that conventional methods for integrating classical equations should be adequate for extended simulations up to 1 ns and that surface hopping agrees semi-quantitatively with wavepacket propagation in the weak-coupling regime. Finally, we describe our optimization of the Newton-X program to reduce computational overheads in data processing and storage.

[1] Mukherjee *et al.* *Philos Trans R Soc A* **2022**, 380, 20200382. (DOI: [10.1098/rsta-2020-0382](https://doi.org/10.1098/rsta-2020-0382))