# Non-adiabatic molecular dynamics approach for simulating nanoscale excited-state phenomena

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Non-adiabatic molecular dynamics (NA-MD), which is a class of methods that simulate the non-adiabatic dynamic based on the trajectory picture, is a useful tool for understanding ultrafast excited-state phenomena. Since NA-MD is grounded on the quantum chemical calculations of excited states, their computational cost is the major obstacle for applying NA-MD to large-scale, complex systems.

To overcome this problem, we have developed computationally efficient NA-MD approaches based on a semiempirical quantum chemical method, density-functional tight binding (DFTB), along with the use of fragmentation approaches called divide and conquer (DC) or patchwork approximation (PA). These schemes were combined with the fewest-switches surface hopping (FSSH)[1,2] and the real-time electron dynamics with Ehrenfest nuclear motion,[3] enabling NA-MD simulations for systems including thousands of atoms with affordable computational cost. These methods were implemented in the developmental version of DCDFTBMD program.[4]

Further, illustrative applications will be presented focusing on coupled electronic and structural dynamics observed in photoexcited states of perovskite solar cell materials,[5] and real-time visualization of charge separation process in the donor–acceptor interface of an organic solar cell (**Fig. 1**).[6,7]

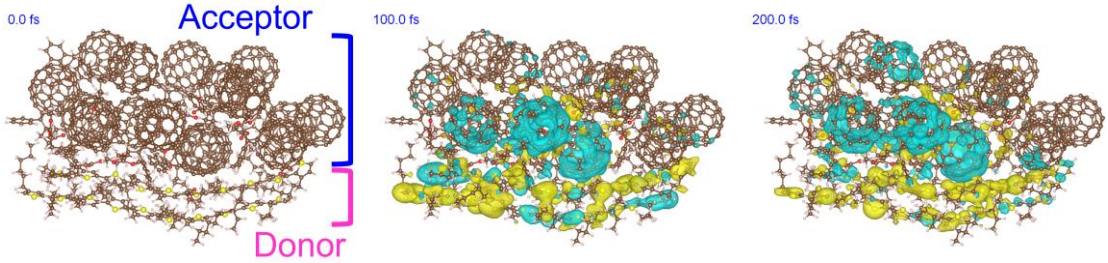


**Fig. 1.** Charge separation dynamics in P3HT/PC61BM interface at the photoexcited state. Yellow and blue isosurfaces represent hole and electron densities, respectively.

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