Non-adiabatic molecular dynamic simulation of the exciton transfer in organic semi-conductors using artificial neural networks.

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June 12, 2023

1 Abstract

Exciton diffusion in molecular aggregates is mainly controlled by the excitonic coupling between the electronic excited states localized on the molecular units. We present an efficient multi-scale model to predict exciton diffusion length from non-adiabatic molecular dynamics simulations in bulk molecular systems. In order to speed up the quantum chemical calculations, we used neural network based models to predict the value of the site energy and exciton coupling of the Frenkel Hamiltonian together with their derivatives, trained on fast longe ranged density functional tight binding (LCDFTB) method. The models are employed to simulate exciton propagation in, few molecular crystal based on fewest-switches surface-hopping approach to calculate the exciton diffusion constant. The results show a good agreement with the experiments.