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**Nonadiabatic electron transfer from conjugated polymer to semiconductor nanocrystal** SVETLANA KILINA, KIRIL TSEMEKHMAN, DMITRI KILIN, OLEG PREZHDO, University of Washington — The photoinduced ultrafast electron transfer from the conjugated polymer (Poly-Phenylene-Vinylene) to the semiconductor nanocrystal (Titanium dioxide / Cadmium Selenide) has been analyzed with nonadiabatic molecular dynamics simulation within classical path approximation. An ab-initio molecular dynamics trajectory is launched for 1ps with initial velocities rescaled to match the room temperature. Nonadiabatic couplings between polymer and semiconductor calculated at each time step are used to construct time-dependent Hamiltonian that drives electron transfer process. The polymer-nanocrystalline composite appears as cost-efficient alternative for traditional Silicon Photovoltaic Cells.

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