

Abstract Submitted
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Photo-induced energy transfer between carbon nanotubes OLENA POSTUPNA, HEATHER JAEGER, OLEG PREZHDO, University of Rochester — The unique structural, mechanical, and electronic properties of carbon nanotubes (CNTs) have recently been attracting significant attention in academic research and industrial applications. Experimental investigation of the physical properties of CNTs is often hindered by questions that can be answered only with rigorous theoretical approaches, such as *ab initio* molecular dynamics. Results of time-domain simulations of energy transfer between photo-excited CNTs are reported. Using a system comprised of a pair of CNTs with different chiralities, (6,4) and (8,4), we elucidate the experimental results obtained by Luer et al [1]. Quantification of adiabatic and nonadiabatic contributions to the transfer process clarifies the mechanism of energy transfer. And, the delocalization of the initial exciton is representative of strong donor-acceptor coupling at high energies. Our work contributes to the ever-growing compendium of energy transfer within nanoscale systems and offers valuable insight toward tailoring CNTs for solar energy conversion.

[1] Larry Luer, Jared Crochet, Tobias Hertel, Giulio Cerullo, Guglielmo Lanzani. *ACS Nano*. Vol.4, No. 7, 4265-4273

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