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Ab initio nonadiabatic molecular dynamics of the ultrafast excitation energy transfer in small semiconducting carbon nanotube aggregates OLENA POSTUPNA, RUN LONG, OLEG PREZHDO, University of Rochester, Rochester, NY — Outstanding physical properties of carbon nanotubes (CNTs), such as well-defined optical resonance and ultrafast nonlinear response, result in CNTs gaining popularity in academic and industrial endeavors as potential effective energy generating devices. Following recent experiments on ultrafast excitation energy transfer in small semiconducting carbon nanotube aggregates [1], we report results of ab initio nonadiabatic molecular dynamics simulation of the energy transfer taking place in two carbon nanotube systems. We investigate the energy transfer between (8,4) and (10,0) CNTs, as well as (8,4) and (13,0) CNTs. In both cases, the CNTs are orthogonal to each other. Luer et al. in [1] elucidate the second excitonic transitions followed by fast intratube relaxation and energy transfer from the (8,4) CNT toward other acceptor tubes. Our project aims to provide a better understanding of the energy transfer mechanism in the given systems, which should foster development of a theory for the electronic structure and dynamics of CNT networks, hence enhancing their tailoring and application in the future. References 1.Larry Luer, Jared Crochet, Tobias Hertel, Giulio Cerullo, Gugliermo Lanzani. ACSNano. Vol.4, No. 7, 4265-4273

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