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Exciton Transfer in Carbon Nanotube Aggregates for Energy Harvesting Applications¹ AMIRHOSSEIN DAVOODY, FARHAD KARIMI, IRENA KNEZEVIC, Univ of Wisconsin, Madison — Carbon nanotubes (CNTs) are promising building blocks for organic photovoltaic devices, owing to their tunable band gap, mechanical and chemical stability. We study intertube excitonic energy transfer between pairs of CNTs with different orientations and band gaps. The optically bright and dark excitonic states in CNTs are calculated by solving the Bethe-Salpeter equation. We calculate the exciton transfer rates due to the direct and exchange Coulomb interactions, as well as the second-order phonon-assisted processes. We show the importance of phonons in calculating the transfer rates that match the measurements. In addition, we discuss the contribution of optically inactive excited states in the exciton transfer process, which is difficult to determine experimentally. Furthermore, we study the effects of sample inhomogeneity, impurities, and temperature on the exciton transfer rate. The inhomogeneity in the CNT sample dielectric function can increase the transfer rate by about a factor of two. We show that the exciton confinement by impurities has a detrimental effect on the transfer rate between pairs of similar CNTs. The exciton transfer rate increases monotonically with increasing temperature.

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Amirhossein Davoody Univ of Wisconsin, Madison

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