

Nanoscale Carbon for Photovoltaic and Therapeutic Applications

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Carbon nanotubes (CNTs), graphene and related materials constitute a new class of systems with many potential applications. We will discuss the results of our recent molecular dynamics (MD) simulations, including both classical MD and state-of-the-art non-adiabatic ab initio MD, aimed at designing photovoltaic devices and drug delivery tools. The first part of the talk will focus on excited state dynamics in CNTs, graphene quantum dots, and photoinduced charge transfer at graphene-TiO₂ interfaces. The second part will discuss the use of CNTs and graphene for intracellular delivery of polar drugs and DNA sequencing.

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