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Heat-Driven Release of a Drug Molecule From Carbon Nanotubes

VITALY CHABAN, OLEG PREZHDO, University of Rochester — Hydrophobicity and ability to absorb light that penetrates through living tissues make carbon nanotubes (CNTs) promising intracellular drug delivery agents. Following insertion of a drug molecule into a CNT, the latter is delivered into a tissue, is heated by near infrared radiation, and releases the drug. In order to assess the feasibility of this scheme, we investigate the rates of energy transfer between CNT, water and the drug molecule, and study the temperature and concentration dependence of the diffusion coefficient of the drug molecule inside CNTs. We use ciprofloxacin (CIP) as a sample drug: direct penetration of CIP through cell membranes is problematic due to its high polarity. The simulations show that a heated CNT rapidly deposits its energy to CIP and water. All estimated timescales for the vibrational energy exchange between CNT, CIP and water are less than 10 ps at 298 K. As the system temperature grows from 278 K to 363 K, the diffusion coefficient of the confined CIP increases 5-7 times, depending on CIP concentration. The diffusion coefficient slightly drops with increasing CIP concentration. This effect is more pronounced at higher temperatures. The simulations support the idea that optical heating of CNTs can assist in releasing encapsulated drugs.

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