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Title and Abstract

Defect-Guided Transport of Biomacromolecules

Defects in the structure of solid-state materials often deteriorate their functional properties yet sometimes, they may grant the materials a new functionality. Graphene, one of the most versatile 2D nanomaterials does not lack imperfections. In fact, one of the most common graphene fabrication procedures - mechanical exfoliation - produces terraced islands of multi-layered carbon sheets. Using all-atom molecular dynamics simulations, here we show that such defects in graphene can be used to direct the transport of adhered biomacromolecules. Our key observation is that, subject to an external force, a single-stranded DNA molecule moves much faster down a step-like defect on a graphene surface than against the defect, and even faster along the defects edge. We find the effect to be robust regardless of the nature of the force used to drive the motion of the biomolecules (mechanical or electrokinetic), the height of the defects or its chemical termination. As a possible practical application of the effect, we demonstrate a system for capturing and transporting a DNA molecule toward a graphene nanopore. Such defect-directed transport can be utilized for building two-dimensional nanoscale highways for precise delivery, concentration and storage of scarce biomolecular species, on-demand chemical reactions and nanopore sensing.