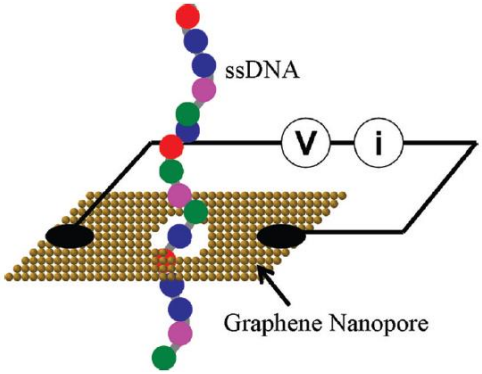
Nanoscale Carbon for DNA Sequencing and Drug Delivery

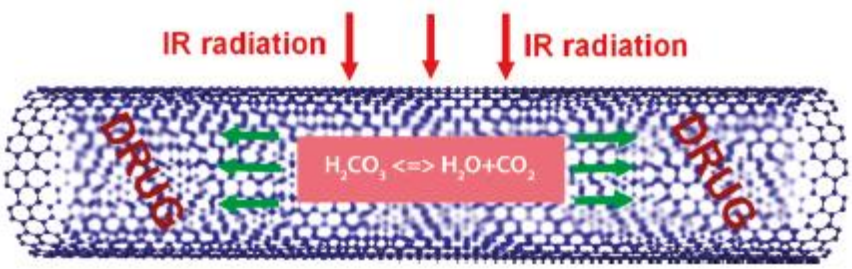
Vitaly V. Chaban, Tammie Nelson, Oleg V. Prezhdo

Departments of Chemistry and Physics, University of Rochester, Rochester, NY 14627, USA

Graphene and carbon nanotubes (CNT) constitute a new class of materials exhibiting unique chemical and physical properties, and leading to new devices and applications. We will discuss our theoretical work aimed at the use of nanoscale carbon in biology and medicine.



We proposed a graphene nanopore device for detecting the base sequence of a nucleic acid [1]. Our ab initio calculations indicate that due to significant differences in the conductance spectra the proposed device has adequate sensitivity to discriminate between different nucleotides. Moreover, we show that the nucleotide conductance spectrum is affected little by its orientation inside the graphene nanopore. The proposed technique may be extremely useful for real applications in developing ultrafast, low-cost DNA sequencing methods.



We investigated the boiling process inside CNTs and showed that confinement substantially increases the boiling temperature and that a small temperature growth above the boiling point dramatically raises the inside pressure [2]. Capillary theory successfully predicts the boiling point elevation down to 2 nm, below which large deviations between the theory and atomistic simulation take place. Considering water droplets, we showed that the ordinary sequence of events with increasing temperature – boiling followed by disappearance of the liquid-vapor boundary at the critical point – is reversed inside CNTs [3]. Precise control over boiling by CNT diameter, together with the rapid growth of inside pressure above the boiling point, suggests a novel drug delivery protocol. Polar drug molecules are packaged inside CNTs [4]; the latter are delivered into living tissues and heated by laser. Solvent boiling facilitates drug release. This work was highlighted in the June 25, 2011 issue of *New Scientist* and other news media.

[1] T. Nelson, B. Zhang, O. V. Prezhdo "Detection of nucleic acids with graphene nanopores: Ab initio characterization of a novel sequencing device", *Nano Lett.*, **10**, 3237 (2010).

[2] V. V. Chaban, O. V. Prezhdo "Water boiling inside carbon nanotubes: towards efficient drug release", *ACS Nano*, **5**, 5647 (2011); highlighted in *New Scientist*.

[3] V. V. Chaban, V. V. Prezhdo, O. V. Prezhdo "Confinement of carbon nanotubes drastically alters the boiling and critical behavior of water droplets", *ACS Nano*, **6**, 2766 (2012).

[4] V. V. Chaban, T. I. Savchenko, S. N. Kovalenko, O. V. Prezhdo, "Heat-driven release of a drug molecule from carbon nanotubes: a molecular dynamics study", *J. Phys. Chem. B*, **114**, 13485 (2010); Journal Cover.