“生物分子在纳通道中的输运及调控”年度报告

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摘 要:为了实现基于纳米孔的低成本超快速DNA测序,需要研究受限空间内聚合物分子的构象机制、摩擦特性,同时要发展流体动力学模型以描述受限空间内生物分子的输运规律。在该年度,我们进一步发展了粗粒化分子动力学模拟模型,开展跨尺度流体动力学建模和计算,并且利用单分子力谱直接探测DNA的单分子界面摩擦力。主要研究结果如下:对DNA分子在石墨烯纳孔和氧化石墨烯纳孔中的穿孔过程进行了研究,发现氧化石墨烯纳孔有可能实现单链DNA分子的逐个碱基过孔;实验研究了多价离子溶液中的纳孔振荡电流信号、离子在纳尺度受限空间中的扩散系数以及低浓度下表面电荷平衡过程对扩散的影响,获得了多个重要结果;进行了纳米颗粒的过孔实验,获得颗粒过孔信号,同时发展了能更准确地预测纳孔介入电阻的理论模型;测量了不同NaCl浓度下DNA的摩擦行为,发现随着浓度增加,DNA摩擦力减少,而DNA在低浓度下显示出较为舒展的构象;发现长链DNA分子具有更舒展的构象,同时链长对DNA摩擦力的影响不大;单分子力谱研究表明,双链DNA在重水和普通水缓冲溶液中的力学稳定性无显著性差异,而双链DNA在甲醇中会自动解螺旋,形成单链DNA。这些研究将加深我们对于DNA等生物分子在受限空间内受力的科学认识,为DNA分子过孔测序技术的发展提供理论依据和设计指导。

关键词:纳米孔 DNA 粗粒化 摩擦力

Annual Report of “Transport and Manipulation of Biomolecules in Nanochannels”

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Abstract: To realize the nanopore-based low cost ultrafast DNA sequencing, it is necessary to investigate the conformation and friction behaviors of polymer and to develop fluid dynamic model to describe the transport of biomolecules in confined space. This year, we further developed the coarse-grained molecular dynamics simulation model to carry out the multiscale modeling and computing of fluid dynamics. The single-molecule interface friction of DNA was directly probed using the single-molecule force spectroscopy. The main results are as follows: The study of the translocation of DNA through graphene nanpore and graphene-oxide nanpore reveals that it is possible to achieve the base-by-base DNA translocation through the graphene-oxide nanopore; Experiments were conducted to investigate the oscillation of nanpore currents in multi-valence solution, diffusion of ions in confined nanochannel and its dependence on surface charge equilibrium, resulting in several important findings; The particle translocation was detected by experimentally measuring the ionic current. Meanwhile, a theoretical model was proposed to predict the access resistance of nanopores; The measurement of fiction of DNA in different NaCl concentrations revealed that DNA friction decreases with the increasing of salt concentration and DNA displays more extended conformation under low salt concentration; It was also found that the long DNA molecule has more extended conformation and the friction is insensitive to the DNA length; The measurements by the single-molecule force spectroscopy showed that the double-stranded DNA has similar dynamic stability in both heavy water and water buffers. However, the double-stranded DNA in methanol will de-helix to form single-stranded DNA. These studies will extend our understanding of forces acting on DNA and other biomolecules in the confined space and provide a theoretical basis and design guide for the development of DNA sequencing techniques.

Key Words: Nanopore; DNA; Coarse grained; Friction

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