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目　录

论　文

Mechanics and Statistics of Bacterial Locomotion

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Abstract: The first part of the talk focuses on the mechanical principle that a single bacterium uses to propel itself. We show that though widely-accepted resistive-force theory qualitatively describes the underlying principle of zero Reynolds number propulsion, it fails quantitatively in the biologically relevant regime due to the negligence of hydrodynamic interactions. In the second part, I will discuss a range of emerging phenomena observed in experimental systems consisting of many bacteria. These phenomena originate from interactions between self-propelled organisms; they include anomalous density fluctuation, scale-invariant correlation, turbulence-like flow pattern, and hydrodynamic clusters.

Coordination of multiple outputs in bacterial chemotaxis

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Abstract: Cells of Escherichia coli are propelled by several helical flagellar filaments, each driven at its base by a reversible rotary motor. When all the motors on a cell turn counterclockwise (CCW), the filaments coalesce into a helical bundle that pushes the cell steadily forward (in a run). When one or more motors switch to clockwise (CW), their filaments come out of the bundle and go through a series of polymorphic transformations (changes in handedness and shape) that result in uncoordinated movement (a tumble) and choice of a new direction for another run [1]. Tumbles are suppressed when cells move up spatial gradients of chemical attractants. Thus, by controlling the direction of rotation of their flagellar motors, cells are able to move toward regions that are more favorable. The central point of regulation in the chemotaxis signaling network is the level of phosphorylation of the diffusible signaling protein CheY (called CheY-P) [2]. CheY-P binds to the motor and controls the motor rotational direction.

In the bacterial chemotaxis signaling network, receptor clusters process input, and flagellar motors generate output [3]. Coordination of these multiple outputs on a cell can be induced by two possible mechanisms: one being the stochastic fluctuation of the intracellular level of the chemotaxis signaling protein CheY-P, the other being extracellular mechanical coupling among bundled flagella.

The motor coordination due to intracellular [CheY-P] (CheY-P concentration) fluctuation has been explored experimentally, by measuring correlation between two motors on a cell with truncated flagellar filaments (thus no coordination due to mechanical coupling among bundled flagella), but the results and the possible mechanisms were still controversial [4 - 6]. The behavioral consequence of this coordination has never been studied experimentally, though there is one theoretical study of the benefits of this coordination due to [CheY-P] fluctuation [7]. The magnitude of motor coordination due to mechanical coupling among bundled flagella has not been studied, neither experimentally nor theoretically.

In the current study, we utilize E. coli strains exhibiting different magnitudes of [CheY-P] fluctuation. We measured their motor behavior by single-motor assays and swimming behavior by 3-d tracking. We experimentally study the behavioral consequence of flagella coordination, and also dissect the relative contributions of these two mechanisms of flagella coordination by correlating motor and swimming behaviors.

Key Words: Bacterial motility, molecular motor, 3-d tracking, bacterial chemotaxis

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Synchronization in growing heterogeneous media

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Abstract : We report results of experiments designed to study the synchronization of a growing heterogeneous system using the dissociated cardiac cultures that consist of both cardiac myocytes（CM） and fibroblast（FB）. We find that there will be aggregation of myocytes to form clusters immediately after plating, followed by a synchronized beatings of cells within the clusters. However, the beatings between the clusters are not correlated in early time but get synchronized only as the cultures mature. The method of principle component analysis is used to analyze the synchronization process. We find that the synchronization of the clusters can be understood by the Kuramoto model of synchronization of coupled oscillators if the coupling constant (K)of the system is considered as a function of time. The experimental results have shown that the value of K is controlled by the growth of the FB. Furthermore, our experimental findings suggest that the overall wave dynamics of the system is controlled by the passive FB in the system.

It is clear that two synchronizations occur during the growth of the cardiac cultures: one for the cells within a cluster which is then followed by synchronization of the cells of the various clusters. These processes would take place only in a heterogeneous system. Since the myocytes in our experiments are thought to be excitable only, it is still not clear whether the myocytes within the clusters are excitable or oscillatory because it is known that the coupling of the passive elements with the active (excitable/oscillatory) elements of the heterogeneous system can lead to a change in the intrinsic dynamics of active elements in the system. Perhaps, this is the origin of the nonmonotonic time dependence of the measured mean frequency, Ω0, found in our experiments. Finally, although it is known that the coupling between FB and CM is through gap junctions, it is puzzling that the FB is growing exponentially, whereas the coupling strength between the clusters is only increasing linearly. Presumably, some other mechanisms must also be involved for the synchronization observed.

Key Words: Cardiac dynamics, Synchronization, coupled oscillators

基于微流控技术的生命软物质研究

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摘要：实际软物质体系如微流体、软体材料及大量生命物质等均存在界面或受限空间，且具有多维尺度、多形态共存和行为复杂等特点，特别是针对受限空间或界面的软物质相关研究面临很大挑战。微流体系统是一种在微米尺度空间对流体进行操控为主要特征的科学技术，近年来发展迅速，为软物质研究、特别是与生命体系相关的生物软物质研究提供了一种重要平台。报告以作者所在研究组的系列工作为基础，以极具发展潜力的微流体系统为核心，着重介绍微流体技术在可控设计、制备多种胶体颗粒软物质、以及生命体系相关软物质研究等方面的应用。主要内容包括：1）基于受限空间的液滴可控形成、定向输运、精确操控等行为研究；2）以受限空间相输运和相变原理为基础，进行具有多响应功能的软物质胶体微颗粒合成与组装研究；3）生命体系相关的细胞和生物体软物质研究复合体系研究，关注受限空间细胞、生物体的生物学行为。

关键词： 软物质，微流体，胶体颗粒，生命体系

Microfluidics-based Platform for Probing the Soft Matters in Limited Space

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Abstract: The actual system of soft matters, such as liquid in microfluidic format, biological existence and bio-interface exhibit a variety of characteristics with multidimensional scale, different morphology and complicated behavior. The complex system requires a suitable platform to study the soft matter with enhanced performance, especially, for the soft matters in biological system and limited space. Microfluidics is the kind of technology which enables to control the small amount of liquid in microchannel at micro-scale, providing a promising platform for the study of soft matters at multiple scales.

This talk will present the various microfluidic platforms established in the author’s lab that can be applied for the researches of soft matters in different ways. The various two-phase droplet behaviors within micro-channels relying on microfluidic control will be described, such as the droplet formation, mixing and micro-valve based accurate handling. In addition, microfluidic based design and controllable synthesis of a variety of soft matters such as colloidal particles and assembly will be presented. The potentials of this technology for the exploration of behaviors of bio-related soft matters, such as cells and organisms in biological system and future opportunities will be discussed as well.

Key Words: Soft matter, microfluidics, colloid particles, life system,

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利用单分子技术探测讯号蛋白的分子机理

谭砚文

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Abstract: Single-molecule fluorescent spectroscopy can provide unique perspectives which complement conventional bulk biochemical approaches. We use single-molecule techniques to illuminate the details of the working mechanism of signaling proteins at different stages of a signalling transduction. Light-sensitive protein cryptochrome plays many different rolls in eukaryotic cells. It is a kind of signalling proteins that is known to retrain circadian clock and involves in the magnetic sensing capabilities of animals. Using smFRET (single-molecule Föster-type resonance energy transfer), we reveal how blue light would initiate in a conformational change in an algae cryptochrome under different redox states and this conformational change is believed to be functionally important. While conformational changes are usually speculated as the cause of activation of signalling function in various receptor proteins, smFRET can afford direct evidence to these hypotheses.

To illuminate the transmission of signals inside cells, we studied the signaling pathway of a plant hormone, Brassinosteroids (BRs). BRs are the plant hormones that involved in numerous plant development processes such as leaf expansion, shoot elongation and pollen tube formation. Once the signal transduction is initiated by the membrane receptor kinase, the downstream signaling pathway is realized by three proteins: BIN2 (brassinosteroid insensitive 2), BES1 (BRI1 ems suppressor1) and a kind of 14-3-3s protein. BRs signaling pathway have been extensively studied via genetics, proteomics, genomics and cell biology techniques. However, these bulk methods can’t follow the transduction process *in situ* or resolve molecular details at a rate matching the true signaling time-scale. Here we use a single molecular assay based on Total-Internally Reflected Fluorescence (TIRF) microscopy to observe the interaction of these three proteins. The result shows that BIN2 can phosphorylate BES1 on the order of seconds, and the dimeric 14-3-3s can only bind with BES1 in its phosphorylated form. In addition, we have, for the first time, found that the interaction between BIN2 and BES1 is oxygen dependent. This result may have implications on BRs signaling pathway’s involvement of stress acclimation in plants.

E-钙粘蛋白和钙粘蛋白 7 亲同相互作用及构型变化的单分子力谱研究

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摘要：有选择性的和强健的细胞粘边在多细胞生物体维持组织结构的完整性和特定的体系结构中起着关键的作用[1,2]。在大多数组织中，细胞粘连是由一类跨膜蛋白，钙粘蛋白，决定的。钙粘蛋白功能失调与肿瘤细胞的侵袭和转移密切相关。钙粘蛋白是一个包含了不同的族和亚族的超级大家庭；其中一类就是经典的钙粘蛋白。E-钙粘蛋白，经典的 I 型钙成员，是上皮细胞的粘连连接的一个重要组成部分，其通过形成圆周形肌动蛋白带来促成细胞的充分极化状态。相反，经典的 II 型钙粘蛋白，比如钙粘蛋白 7，则表现出显著弱的粘连，并主要在间质组织中出现[3]。I 型和 II 型钙粘蛋白分子都有类似的组织构成[4]：一个胞质区域，一个跨膜区和一个胞外区。它们的胞外区都有着类似的三维结构：包括五个串联重复域，称为细胞外钙粘蛋白（EC）域。每个 EC 域由约 110 个氨基酸组成，形成了七 β-链，并组成两个β-片。晶体学数据显示在体外经典 I 型钙粘蛋白亲同相互作用可以形成 X-二聚体和链交换式二聚体，而 II 型钙粘素也发现能形成类似的链交换二聚体。

然而，虽然相关的文献众多，但是到目前为止我们对于控制钙粘蛋白识别和粘合强度的机制也仅仅是部分的了解。因此，本报告中，我们利用原子力显微镜（AFM）和磁镊直接在分子水平上比较细胞外（EC）域的 E-钙粘蛋白（I 型）和钙黏蛋白 7（II 型）的亲同相互作用和机械稳定性。我们发现，即使胞质区域缺失，相比于钙粘蛋白 7，E-钙粘蛋白仍显示了较大的解离力。同时，还发现外部施加的力的 AFM 悬臂能增强 E-钙粘蛋白的相互作用，但对钙粘蛋白 7 的相互作用增强不明显。此外，EC 域解折叠实验的结果表明，钙粘蛋白 EC 域的稳定性并不能够在其亲同相互作用断裂前仍保证 EC 域的完整性，因此部分的解折叠/构型变化的可能性是不可忽略的。此外，磁镊子实验表明，部分解折叠 EC 域所需的力与在体内由骨架产生的力已经比较接近。基于这些研究结果，我们提出了另一个机理来强化钙粘蛋白介导的细胞粘连：这可以解释 X-二聚体相链交换二聚体的转化，以及 I 型和 II 型钙粘蛋白粘合性能的不同。这样，我们第一次从一个全新的角度来探索钙粘蛋白介导的细胞粘附机制。这种机制可能与其他观察到的机制共同在生物体内起到作用。

关键词：力谱，细胞粘连，钙粘蛋白，原子力显微镜，磁镊子

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Homophilic Interaction and Deformation of E-cadherin and Cadherin 7 Probed by Single Molecule Force Spectroscopy

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Abstract: Selective and robust cell-cell adhesion plays a key role in maintaining tissue structural integrity and specific architecture in multicellular organisms. In most tissues, cell-cell adhesion is dominated by a class of transmembrane proteins named cadherins. Dysregulation of cadherin function correlates with tumor cell invasion and distant dissemination. The cadherin superfamily comprises distinct families and subfamilies; one of these is the classical cadherins. E-cadherin, the prototypic member of classical type I cadherins, is an essential component of epithelial adherens junctions and contributes to a fully polarized state in the cell through the formation of a circumferential actin belt. In contrast, classical type II cadherins, such as cadherin 7, show significantly weaker adhesion and are mainly expressed in mesenchymal tissues. Type I and type II cadherins demonstrate similar domain organization: a cytoplasmic region, a transmembrane region, and an extracellular region. The extracellular segments of type I and type II cadherins share a similar 3D structure that comprises five tandem repeats, called extracellular cadherin (EC) domains. Each EC domain consists of about 110 amino acids forming seven β-strands that are organized into two β-sheets. Crystallographic data suggest the formation of X-dimers and strand-swapping dimers by the homophilic interaction of classical type I cadherins in vitro, while type II cadherins are also found to form similar strand-swap dimers.

However, mechanisms controlling cadherin recognition and adhesive strengthening are only partially understood so far. Here, we used atomic force microscopy (AFM) and magnetic tweezers to direct compare the extracellular (EC) domains of E-cadherin (type I) with that of cadherin 7 (type II) at the molecular level by investigating the homophilic interactions and mechanical stability. We found that even in the absence of the cytoplasmic region, E-cadherin displays a stronger unbinding force than cadherin 7. External forces applied by the AFM cantilever were also found to strengthen the E-cadherin interactions rather than the cadherin 7 interactions. In addition, the results from the unfolding experiments suggest that the stability of cadherin EC domains are not enough to ensure their integrity prior to the rupture of their homophilic interaction, and thus the chance of partial unfolding/deformation of these EC domains is not negligible. Furthermore, magnetic tweezers experiments demonstrated that partial unfolding of EC domains can take place at a force close to that borne by the cytoskeleton in vivo. Based on these findings, we proposed an additional strengthening mechanism of cadherin-mediated adhesion, which can explain the transformation of X-dimers into strand-swapping dimers, as well as the distinct adhesive properties between type I and type II cadherins. This is the first attempt from such a perspective to ascertain the mechanisms of cadherin-mediated adhesion. This mechanism may work in vivo together with other observed mechanisms.

Key Words： force spectroscopy, cell adhesion, cadherin, atomic force microscopy, magnetic tweezers

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弯曲鞭毛的集体行为：自组装漩涡结构

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摘要:长棒形物体作类似正弦形状的蛇行运动在自然界中很常见，例如高等动物的精子尾部鞭毛的摆动，又如一些线虫的蠕动等。这种运动方式使个体在非常黏滞的低雷诺数流体环境中仍能有效地运动。当长棒形粒子除了正弦摆动外还有额外的自发曲率时，粒子的轨迹呈环形。不同于作直线运动的长棒形粒子的集体行为【1】，环形轨迹的长棒形粒子体系可自组装形成漩涡阵列结构【2】。

我们模拟了二维下作正弦摆动的弯曲鞭毛体系。不可穿透的鞭毛处于各向异性的摩擦力环境中，通过正弦形状的摆动获得推进力，并且其质心在二维平面中作顺时针运动轨迹。体积排除作用是长棒形的鞭毛间的唯一相互作用，它造成的向列型相互作用使鞭毛倾向于作同心圆周运动。当体系的鞭毛浓度足够时，多根鞭毛组装成顺时针旋转的漩涡，并且体系中总是存在多个漩涡。

这些漩涡的直径 D_v 正比于鞭毛的自发轨迹的直径 D_0，并轻微地依赖于体系的鞭毛密度，但与鞭毛的摆动频率的分散度不相关。受鞭毛游动速度的限制，单个漩涡内部的旋转角速度 ω 总体呈 R^{-1} 衰减，R 为至漩涡中心的距离。鞭毛沿径向的分布概率密度函数为双峰型。与无体积排除效应的点状环形运动粒子体系所形成的液态漩涡阵列略有不同【2】，鞭毛漩涡的阵列表现出近程的六角晶格排列，而远程仍然是液态分布。

我们的结果与海胆精子实验中所见的自组装漩涡阵列一致【3】。可见在这种弯曲长棒状自推进粒子的集体行为中，体积排除是一种重要的相互作用，可直接导致漩涡结构的形成并决定漩涡的各种性质。

关键词: 自推进粒子，自组装漩涡，鞭毛

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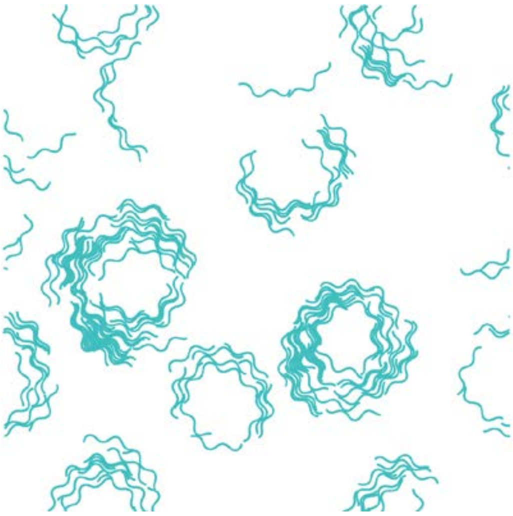

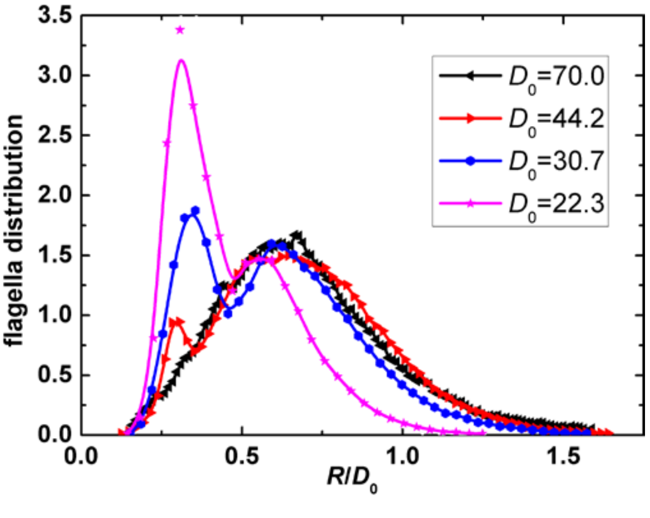
3.5
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0.0
flagella distribution
0.0
0.5
1.0
1.5
R/D_0
D_0=70.0
D_0=44.2
D_0=30.7
D_0=22.3

Fluctuation and fidelity control in T7 RNA polymerase transcription elongation

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Abstract: Polymerases are essential enzymes responsible for gene replication or transcription. A polymerase moves along DNA or RNA while synthesizing a new strand of nucleic acid, largely according to Watson-Crick base pairing with a template strand. A polymerase not only catalyzes the polymerization reaction but it also increases the fidelity. We first examined kinetically the stepwise selections in an elongation cycle of the polymerase, with a controlled differentiation free energy between the right and wrong nucleotide at each selection checkpoint. It is found that early selection is essential to achieve an efficient fidelity control, and an initial screening is indispensible for maintaining the speed high. Overall, the elongation error rate can be repeatedly reduced through multiple selection checkpoints [1]. Our previous kinetic modeling work on T7 RNA polymerase (RNAP) suggested that a small post-translocation free energy bias stabilizes Tyr639 in the active site to aid nucleotide selection [2], based on single molecule experiments. The free energy bias slightly modulates Brownian ratcheting of T7 RNAP, in which nucleotide insertion serves as a pawl to prevent backward translocation. Recently, we performed atomistic molecular dynamics (MD) simulations that demonstrate that Tyr639 is stabilized marginally by associating with the end base pair of the DNA-RNA hybrid at post-translocation. Pre-insertion of a right RNA nucleotide for base pairing with the template does not enhance the Tyr639 stabilization. Pre-insertion of a wrong nucleotide, however, substantially stabilizes Tyr639 further in the active site. In particular, a DNA nucleotide strongly enhances Tyr639 stacking with the end base pair, while a base mismatched nucleotide tightly grabs on Tyr639. Since full insertion of the nucleotide requires Tyr639 to move out of the active site, the residue plays a critical role in selectively gating the right nucleotide and thus ratcheting the polymerase for elongation [3]. Furthermore, we find that the strong stabilization of this residue in the active site is disrupted in the mutation of Tyr639 into Phe639 upon a DNA nucleotide pre-insertion. The finding explains the reduced differentiation between ribo- and deoxyribonucleotides that has been recorded experimentally for the mutant polymerase.

Keywords: polymerase, fidelity control, kinetic modeling, molecular dynamics simulation, Brownian ratchet

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预测 RNA 三维结构、稳定性及其离子效应的粗粒化模型

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摘要：RNA 是重要的生物分子，执行着遗传信息的储存、传递以及基因调控等功能[1]。RNA 的重要功能与其复杂的空间结构及结构变化紧密相关，然而由于局限性而且成本昂贵，实验上测得的 RNA 结构数据还相对较少。因此，基于物理原理的 RNA 结构预测对 RNA 生物功能的理解和应用具有重要意义[2-4]。RNA 结构强烈依赖于溶液的温度和离子条件[5-7]，为了预测 RNA 三维结构、稳定性及其离子效应，我们建立了基于 Monte Carlo 的粗粒化结构预测模型。模型中，每个核苷酸由三个粗粒化的球代表，分别处于 P、C4’及 N1 或 N9 原子位置，其力场由 PDB 数据库提取的经验势和热力学的实验测量值得到。对于 46 个 RNA 分子（≤45 nt），此模型成功预测了其近天然态三维结构，平均 RMSD 为 3.5Å；对于 30 个 RNA 发夹分子，此模型所预测的溶解温度与实验一致，平均相差 1.1℃；对于 6 个 RNA 发夹分子在广泛[Na^+]范围溶解温度的预测也与实验吻合，平均相差 0.9℃。此模型将为预测复杂的大 RNA 结构、稳定性以及高价离子效应奠定重要基础。

关键词: RNA 结构预测，稳定性，离子效应，粗粒化模型

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Modeling Mechanical Properties of DNA: Allosteric Protein Binding, Loop Formation, and Longitudinal Fluctuations

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Abstract: The deformability of DNA has great impacts on its overall shape as well as on many biological functions, such as protein-DNA binding, chromosomal DNA packaging, DNA damage repair, and regulation of gene expression. Here we present our recently developed coarse grained mechanical model of DNA that studies the local deformations of DNA from its canonical structure. In collaboration with recent experimental studies, the correlation between local deformations is unveiled and identified as the underlying mechanism for the observed allosteric protein binding. This newly discovered correlation improves our understanding of the flexibility of DNA and suggests modification of the traditional description of DNA as an elastic rod, which is valid only for long DNA chains and has been challenged by recent experimental studies at shorter length scales. With explicit consideration of the length scale over which local deformations are correlated, our improved model predicts a length dependent flexibility. While our model reduces to the traditional worm-like chain model in the long chain limit, it predicts that DNA becomes much more flexible at shorter sizes that are of biological importance, in good agreement with recent loop formation measurements of short DNA fragments around 100 base pairs.

Atomistic simulations of peptide aggregation and nanoparticle inhibition

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Abstract The pathogenesis of neurodegenerative diseases such as Alzheimer's disease (AD) and type II diabetes is associated with the abnormal self-assembly of the related peptide into toxic β-sheet-rich aggregates. The inhibition of β-sheet formation has been considered as the primary therapeutic strategy for neurodegenerative diseases. In spite of extensive experimental studies, the atomistic structures of amyloid oligomers and the aggregation mechanism remains elusive. In this talk, I will present our molecular dynamics simulation results on the aggregation of different fragments from Alzheimer's amyloid-β peptide (A□), human islet amyloid polypeptide and tau proteins. The effect of nanoparticles on peptide aggregation is also discussed. The results can not only enhance our understanding of the molecular mechanism of peptide aggregation, but also will provide novel insights into the development of drug candidates against amyloidosis.

Key Words： amyloid fibril, oligomer, β-sheet formation, free energy landscape, inhibition mechanism, hydrophobic/aromatic-stacking interaction, replica-exchange molecular dynamics simulations.

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The neural circuit and synaptic dynamics underlying perceptual decision-making

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Abstract: Decision-making with several choice options is central to cognition. To elucidate the neural mechanisms of multiple-choice motion discrimination, we built a continuous recurrent network model to represent a local circuit in the lateral intraparietal area (LIP), which is considered to be a neural correlate of perceptual decision-making. The model is composed of 2048 pyramidal cells and 512 interneurons. Both types of neurons are directionally tuned, and their preferred directions separately cover a full circle uniformly. All neurons are reciprocally connected. The synaptic connectivity strength depends on the difference in preferred directions between neural pairs except the interneuron-to-interneuron connectivity is uniform. This is in sharp contrast to homogeneous connectivity between pyramidal cells and interneurons in previous models. Specifically, we assume two types of inhibitory connectivity: opposite-feature and similar-feature inhibition, representing that the connectivity strength has a maximum between neural pairs with opposite and identical preferred directions, respectively.

We followed the experimental protocol and characterized the spatiotemporal firing pattern of the network on a multiple-choice motion-discrimination task. With a common parameter set, the model accounted for a wide variety of physiological and behavioral data from monkey experiments, including those that previous models failed to reproduce. The main results are as follows. (1) The network is endowed with slow excitatory reverberation, which subserves the buildup and maintenance of persistent neural activity, and predominant feedback inhibition, which underlies the winner-take-all competition and attractor dynamics. (2) The opposite-feature and opposite-feature inhibition have different effects on decision-making. The former endows the decision-making circuit with an elimination strategy, which effectively reduces the number of choice alternatives for inspection to speed up the decision process at the cost of decision accuracy. Conversely, the latter markedly enhances the ability of the network to make a choice among multiple options and improves the accuracy of decisions, while slowing down the decision process. A simplified mean-field model was also presented to analytically characterize the effect of structured inhibition on fine discrimination. (3) We made a testable prediction: only the combination of cross-feature and similar-feature inhibition enables the circuit to make a categorical choice among 12 alternatives. Together, the current work highlights the importance of structured synaptic inhibition in multiple-choice decision-making processes and sheds light on the neural mechanisms for visual motion perception.

Key Words: Continuous recurrent network model, fine discrimination, motion discrimination, random-dot display, structured synaptic inhibition

Reference:

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Optimal microdomain crosstalk between endoplasmic reticulum and mitochondria for Ca2+ signaling

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Abstract: the calcium ion (Ca^{2+}) is a ubiquitous intracellular signal controlling diverse cellular functions. It has been widely accepted that the inositol 1,4,5-trisphosphate receptors (IP_3R) function as Ca^{2+} release channels on the endoplasmic reticulum (ER) membrane. Since the 1990s, the manner in which mitochondrial Ca^{2+} uptake through mitochondrial Ca^{2+} uniporter (MCU) shapes intracellular Ca^{2+} signaling has attracted much attention. The key questions presently debated are: to what extent mitochondria acquire Ca^{2+}; what impact mitochondria have on cytosolic Ca^{2+} signals; and what dimensions the ER/mitochondria Ca^{2+} microdomain might have. To address these questions, we constructed a Ca^{2+} signaling model to consider the Ca^{2+} crosstalk within microdomains between IP_3Rs and MCU. Our model predicts that there is a critical IP_3R-MCU distance at which 50% of the ER-released Ca^{2+} is taken up by mitochondria and that mitochondria modulate Ca^{2+} signals differently when outside of this critical distance. The model demonstrates the existence of an optimal IP_3R-MCU distance (30-85 nm) for effective Ca^{2+} transfer and the successful generation of Ca^{2+}-signals in healthy cells. This study highlights the importance of the IP_3R-MCU distance on Ca^{2+} signaling dynamics.

肌肉蛋白 titin 的免疫球蛋白结构域在恒定拉力下的平衡态折叠/去折叠转变

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摘要：肌肉蛋白 titin 在拉力下的折叠/去折叠转变直接影响肌肉的弹性和功能调控，titin 已经被单分子操纵实验（特别是原子力显微镜）所广泛地研究。因为自然状态和去折叠状态之间存在很高的能垒，这使得通常需要超过 100 pN 的拉力才能使其在若干秒钟的时间尺度内完成去折叠转变。而在临界拉力下，即在折叠速率和去折叠速率相等的拉力作用下，蛋白质去折叠和折叠的速率都非常的慢，无法在原子力显微镜所容许的时间尺度内完成测量。这使得利用原子力显微镜直接测量其依赖于拉力的平衡态折叠自由能很难被实现。

我们应用自主搭建的超级稳定的磁镊单分子操纵设备，对 8 个 titin I27 重复结构域的蛋白质进行了测量。通过对单个蛋白在恒定拉力下长时间的稳定测量我们得到了不同拉力下的平衡态折叠自由能，确定了 titin I27 的折叠/去折叠临界拉力为 5.2 皮牛，同时直接测量得到了拉力依赖的蛋白质折叠速率。我们的实验技术和理论框架可以被用来研究更多的不同类型的蛋白质的折叠/去折叠过程，自由能曲面，力学传感功能等。

关键词：titin，I27，折叠，去折叠，磁镊

碳纳米颗粒曲率在其结合蛋白质时的影响

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摘要：作为新兴科技中的一颗明星，纳米材料在诸如：基因传递、细胞内成、肿瘤治疗以及生物实验技术等各种重要的生物技术领域都具有广泛的应用前景。与此同时，这些纳米生物料本身的安全性问题，以及它们与生物系统的相互作用也引起了广泛的关注。我们使用分子动力学方法模拟蛋白质结构域与各种碳纳米颗粒相互作用的过程。从而在分子的尺寸来研究纳米颗粒中可能存在的毒性机理。我们之前的研究已表明，碳纳米颗粒能以不同的方式与蛋白质结合，从而影响蛋白质的功能。而且在蛋白质与碳纳米颗粒的相互结合的过程中，蛋白质中的疏水残基与碳纳米颗粒的疏水相互作用，以及芳香残基与碳纳米颗粒表面的六元环之间的π堆积相互作用起了主要的贡献。最近我们进一步的使用分子动力学模拟研究了蛋白质与富勒烯、碳纳米管与石墨烯三不同的纳米颗粒之间的相互作用的过程。虽然π堆积相互作用的相互作用能较大，但是碳纳米颗粒表面的曲率能影响残基与碳纳米颗粒相互作用的熵，并通过对熵的影响来调节这两种相互作用力的在结合中的贡献，使得疏水相互作用在曲率较大的碳纳米管与蛋白质相互作用中作主要贡献，而π堆积相互作用在曲率较小的石墨烯中作主要贡献。

关键词：蛋白质构象、碳纳米颗粒、π堆积相互作用、疏水相互作用、曲率

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二维纳米粒子跨细胞双层磷脂膜输运的计算机模拟及理论分析

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摘要：研究具有复杂拓扑结构的功能纳米粒子夸细胞膜输运的动力学路径及机理对于明晰其细胞毒性，进而研制新型高效靶向药物输运体系来说具有重要的理论和实际意义。然而，囿于极小的空间尺度和极短的时间尺度，很难单纯通过实验研究来解决此问题。计算机模拟和基于膜弹性理论的理论分析方法因而成为洞悉该过程的有效途径。针对此问题，本课题组采用介尺度模拟和理论分析相结合的方法，开展了对树枝状大分子和两维石墨烯纳米片跨细胞膜输运的计算机模拟和理论分析。【1-5】本论文即集中介绍我们在石墨烯及其衍生物跨细胞膜输运的动力学路径及机理方面的一些理论和模拟研究工作，着重强调其跨膜输运过程的路径和机理对于膜张力，石墨烯尺寸和氧化程度以及膜的受体蛋白等因素的依赖性。通过运用介尺度计算机模拟，我们揭示了石墨烯纳米片与膜作用时的多种独特状态，例如：三明治结构，半球胶束结构，刺穿结构以及膜受体介导的石墨烯表面膜滑移结构等；同时借助基于膜弹性的 Canham-Helfrich 理论对该过程中的能量变化进行了详细计算和理论分析，阐明了这些不同的状态所对应的跨膜输运动力学路径及其发生的难易程度。最近，通过系统的计算机模拟和理论分析，我们进一步阐述了膜受体蛋白对于石墨烯二维纳米片跨膜输运的影响，发现了一些比较新奇的现象。这些工作对于揭示石墨烯等两维纳米材料潜在的细胞毒性，进而理解其对人体健康的危害性，以及在纳米医学等领域的深入应用具有比较重要的促进作用。

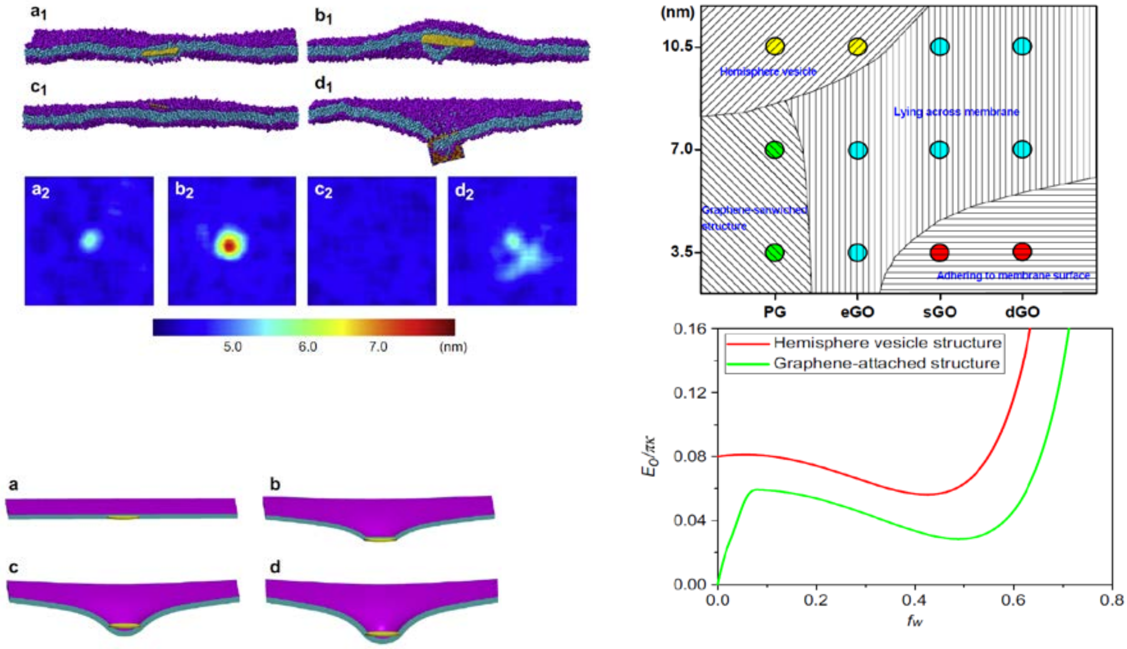

图 1. 部分模拟和理论分析结果

关键词：二维纳米粒子，跨膜输运，石墨烯，动力学路径，理论分析，计算机模拟

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核糖开关的调控机制

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摘　要: 核糖开关是 mRNA 上能够与自由代谢产物或其他小分子配体结合或由于环境条件变化而引起构象变化从而调控目的基因表达的 RNA 结构元件【1-2】。迄今已在细菌，真菌，植物动物中发现了多种核糖开关的存在，一般位于受控基因的非翻译区或者高等动物内含子区，包含适体域和基因表达单元【3】。核糖开关主要有两种调控机制：调控转录提前结束和调控翻译的开始，除此之外，核糖开关还可以调控 mRNA 的剪切等生物过程【4】。核糖开关调控过程涉及很多生化过程的精确协调，如 RNA 折叠、转录延伸、代谢物结合、螺旋形成、核糖体结合以及 mRNA 加工等。由于转录过程中构象切换的动态过程无法确定，导致核糖开关调控基因表达的具体细节并不是很清晰。我们建立 RNA 二级结构宏观动力学方法，能成功处理长链长时间的折叠和转录动力学问题【5-8】。采用此方法我们研究了结合 adenine (A), S-adenosylmethionine (SAM), flavin mononucleotide (FMN)三类常见的核糖开关，给出了在不同条件下（转录速率，暂停，配体浓度）的转录折叠行为。结果显示 addA 和 yitJ 核糖开关可以在转录结束之后根据配体浓度来选择开关状态。相反，对于对于动力学调控的 FMN 和 pbuE 核糖开关，其下游基因的表达依赖于转录过程；降低转录速率或者适当的暂停可以有效地促进配体与 RNA 的结合所对应生物功能的实现。这些结果反映了核糖开关的不同调控机制，为以后基因功能研究、生物传感器和新型抗菌药物的设计提供理论基础。

关键词: 核糖开关，转录折叠

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Single polymer compact reveals the dissociation force of catechole-Fe3+ complex

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Abstract: Growing evidence has proved that metal-ligand coordination plays an important role in the life process of marine creatures. Coordination between Fe3+ and catechol ligands, which was first investigated in mussel byssal threads, has recently correlated to the adhesive and cohesive ability of most marine creatures. Pioneer work has revealed that the stoichiometry of catechol-Fe3+ complex (mono-, bis- and tris-) is triggered by pH during the deprotonating process of catechol hydroxyls, thereby further affect the performance of the hardness and extensibility of the cuticle of marine creatures and is proposed to endow self-healing properties. However, the strength of catechol-Fe3+ bond and the Fe3+ concentration impact, another two crucial factors of catechol-Fe3+ ligand, has still been unknown. To figure out the strength of catechol-Fe3+ ligand, we used hyaluronic acid (HA) modified with DOPA mixing with FeCl3 solution to form HA-DOPA-Fe3+ assembly via catechol-Fe3+ bond. By changing the concentration of Fe3+, we can make clear that the influence of the amount of Fe3+. Thanks to single assembly force microscopy based on atomic force microscope method, we found that the strength of bis-catechol-Fe3+ ligand is around 200 pN, and the tris-catechol-Fe3+ ligand is around 110 pN. We also revealed that the Fe3+ concentration could modulate the mono-, bis- and tris-complex, which were confirmed by UV-Vis spectra and Raman spectra. To provide molecule-level insights into the metal-coordination bond cleavage process, a first-principles study of mechanical response of bis- and tris-catechol-Fe3+ complexes is implemented in this work. Fig. f (a) shows the optimized ground state geometries for bis- and tris- catechol-Fe3+complexes. The bis-complex is shown to prefer a planar square structure while the tris-complex intends to occupy a non-planar octahedron configuration. We verified that the characteristics of these calculated structures and their electronic absorptions are in close agreements with experimental findings. Our findings gave abundant information on the chemical nature of catechol-Fe3+ ligand and provide useful guidance for designing new generation biomaterials.

Key Words: Mussel foot protein, DOPA, AFM, single micelle force spectroscopy

应用光镊捕获活体动物体内的红细胞

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摘要：由于动物体内环境的复杂性，在体外或培养环境下的生物学研究不一定能够准确反映在体内的生物学活动，因此活体生物体内检验是生物学研究的最终验证。在活体动物体内研究操控细胞，对生命科学、医学研究等领域具有重要意义。鉴于激光的穿透性质，光镊可以进入生物组织内部，能实现体内的细胞操控。

我们利用多年发展的光镊技术，首次对活体动物内的细胞实现光学捕获。研究表明，光镊可以直接深入到活体内，对细胞进行有效操控。用光镊穿过小鼠耳朵真皮层，到达深度约 50 微米毛细血管中，捕获和操控血管中的红细胞。将光镊固定在血管中心，血管中快速流动的细胞经过光阱时被逐渐减速，直到一个细胞停留在光阱中，光镊将细胞捕获，并实现了三维操控。在应用方面，利用光陷阱的作用聚集红细胞，人为制造血管堵塞。另外对血管中已聚集的细胞团簇，拖拽其中一个细胞引导疏通，使聚集的细胞逐渐疏散开，恢复正常血液流动，实施非接触手术式的血管疏通。

另外，我们还对该技术进行了进一步的研究，研究结果包括通过球差修正技术，使得水浸物镜能够捕获体内细胞；通过适当压缩光束直径增强光阱横向捕获力；采用矢量光束作为捕获光源，增强光阱纵向捕获力。

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关键词：光镊，活体动物体内，捕获与操控

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Mapping Intracellular Diffusion Distribution Using Single Quantum Dot Tracking

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Abstract: The crowded intracellular environment influences the diffusion-mediated cellular processes, such as metabolism, signaling and transport. The hindered diffusion of macromolecules in heterogeneous cytoplasm have been studied over years, but the detailed diffusion distribution and its origin still remain not very clear. Here, we introduce a novel method to map rapidly the diffusion distribution in single cells based on single-particle tracking (SPT) of quantum dots (QDs). The diffusion map reveals the heterogeneous intracellular environment and, more importantly, an unreported compartmentalization of QD diffusions in cytoplasm. Simultaneous observations of QD motion and GFP-tagged endoplasmic reticulum (ER) dynamics provide direct evidence that the compartmentalization results from micron-scale domains defined by ER tubules, and ER cisternae form perinuclear areas that restrict QDs to enter. These results shed new light on the diffusive movements of macromolecules in the cell, and the mapping of intracellular diffusion distribution may be used to develop strategies for nanoparticle-based drug deliveries and therapeutics.

利用光镊单分子检测驱动蛋白动力学特性

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Abstract： Kinesin family plays some important roles within a cell society. We used optical tweezers to investigate kinesins include Kinesin-1(K560) and Kinesin-7(CENPE). Based on a DIC microscope, the optical trap have a non-symmetrical stiffness distribution. Through coordinate rotation of detected signals, we can measure movements dependent on external force for motor protein moving along microtubule with arbitrary orientation. The measurements of K560 were in accord with reported results in single molecule chareristics. However, CENPE moved along microtubule slowly. Under inhibition of SUK4, its movements appeared stuck state. Occasionally, the stuck situation can be broken, then, the protein moved on. When increasing the molecule binding concentration, two or more molecules of CENPE moved slower than single molecule. Meanwhile, the elasticity of CENPE had been measured by detecting velocity of trapped beads relative to fixed beads when piezo-stage moving. The single molecule chareristics of CENPE are vital to chromosomes moving to metaphase plate and subsequent oscilllation.

关键词：光镊；驱动蛋白；单分子检测；CENPE；

活性氧(ROS)自由基导致 DNA 碱基损伤机制的理论研究

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摘要：宇宙(太空)辐射、核辐射、粒子辐射及电离辐射对生物大分子的损伤导致 DNA 基因突变、蛋白质变性、细胞癌变乃至生命体系的崩溃。[1-3] DNA 损伤是各种辐射生物效应的物质基础，与自由基的作用密切相关，特别是活性氧(ROS)自由基在其中起着关键作用。为了深入理解辐射导致 DNA 损伤现象，本工作采用密度泛函(DFT)和二阶微扰理论(MP2)对 ROS 自由基与 DNA 碱基(对)的反应性进行了理论研究，旨在揭示 ROS 自由基导致 DNA 损伤的机理和反应规律，同时寻找一种合理有效的方法来研究 ROS 自由基与真实溶剂环境下的 DNA 之相互作用。结果表明：（1）通过对 T、C、G、A 的加成和抽氢反应的研究证实了 G 和 T 对接受·OH 攻击的敏感性明显强于 A 和 C；（2）“虚拟溶剂模型(ISM)”中，即使溶剂是极性的，溶剂效应对·OH 与 DNA 碱基的相互作用没有重大贡献；而“真实溶剂模型(ESM)”中的水会因为氢键网络的形成严重干扰·OH 与 DNA 碱基的反应；（3）比较分析·OH、氢过氧(·OOH)和超氧阴离子(O_2^{-}·)三种 ROS 自由基攻击胸腺嘧啶(T)的反应，说明·OH 对 DNA 的破坏性更强。

关键词： 羟基自由基，DNA 损伤，DFT 理论

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Theoretical Investigation of the Mechanism of DNA Damage Induced by ROS Radicals

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Abstract：All kinds of radiations, including cosmic (space) radiation, nuclear radiation, par-ticle radiation, and ionizing radiation induced the damage of biomacromolecule such as mutagenesis, protein denaturation, carcinogenesis, cell aging and even lethality of life. The basis of the biological effects brought by radiations is the DNA damage, which is closely related to free radicals, especially reactive oxygen species (ROS) free radicals. In order to better understand the damage of DNA induced by radiations, density functional theory (DFT) and the second order Møller Plesset perturbation theory (MP2) are used to study the reactivity of DNA bases (pairs) in the presentence of ROS radicals. The aims of this investigation are to discovery the mechanisms of the reactions be-tween ROS radicals and DNA bases (pairs), and to find a reasonable way for probingthe interactions of ROS radicals with DNA in solvents. These results suggest that G and T have higher reactivity towards the reaction with ·OH than A and C, i. e., hydroxyl radicals is most likely to attack T and G bases. In addition, the solvent effects does not favor the reactions between ·OH and T in implicit solvation model (ISM), even in polar solvents. When using explicit solvation model (ESM), the dehydrogenated reactions are interfered by the formation of hydrogen bonds. By comparing the reactions between the three ROS free radicals and thymine, i.e., ·OH, perhydroxyl radicals (·OOH) and superoxide anion radicals (O2-·), ·OH is proposed to be the most destructive species toward the DNA damage.

Key Words：Hydroxyl radicals, DNA damage, DFT

校对机制对提高 DNA 复制保真度的理论分析

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摘要：DNA 复制是个精确调控的生化酶促过程，许多 DNA 聚合酶能将复制的出错率控制到 10^{-7} 到 10^{-8} 量级。这些 DNA 聚合酶，如 Polymerase I（Pol I），大都同时具有聚合和剪切两个位点，剪切位点可以将错配的核苷酸切掉来降低聚合的出错率，起到一个校对的功能。剪切位点校对作用的存在，对 Pol I 的保真度有数个数量级的贡献[1]。关于校对机制如何提高 Pol I 的保真度，目前还没有一个完整的理论模型。由于 DNA 先导链的 3’端可以在聚合和剪切位点可逆转移，我们在主方程的框架内，基于化学反应动力学，建立了一个末端可以在两态之间转变的聚合-校对生长模型。在对此模型的化学反应通路的几种拓扑结构的初步分析中，我们发现末端的两态之间的存在至少一个中间态对保真度的提高是必要的。这进一步支持了近年来实验上对 Pol I 聚合和剪切两态之间中间态的存在的发现[2]。该理论不仅可以对剪切位点如何提高 Pol I 的保真度进行一定的解释，更重要的是，还有助于从分子设计的层次上理解 Pol I 的校对工作机制。

关键字：DNA 复制　保真度　校对　剪切位点

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DNA 双链的非均匀力学模型

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摘要：众所周知，DNA 双链是生物信息的主要载体。而容易被忽视的是它作为一种物理结构在不停地承受歪曲或扭转。实际上，较短 DNA 双链（<100 nm）的弯曲在 DNA 储存与基因调节中扮演关键的角色。比如，被 DNA 双链所缠绕的核小体是染色体的基本单位，其直径仅为 10nm。因此，较短 DNA 双链的弯曲刚度或者与之等效的持续长度是非常重要一个物理量。传统的观点认为 DNA 双链可被简化为一均匀的各向同性的弹性杆，其力学行为可以用蠕虫状链模型描述，持续长度约为 50nm。但是，最近一些先进实验技术的数据却说明这种观点是不正确的，很短的 DNA 双链持续长度比 50nm 小得多。DNA 双链的横截面在结构上是非均匀的。双链的骨架是亲水的，分布在外围包裹着在链与链之间所形成的疏水的相互作用。根据这一结构特点，我们建立了 DNA 分子的复合材料力学模型，并把剪切滞后理论推广用于分析 DNA 在热扰动下所表现出的持续长度。理论分析表明，当 DNA 双链之间的相互作用比较弱时，DNA 的持续长度出现反常行为。很短的 DNA 双链持续长度比较小，持续长度随着 DNA 长度增加而变大，直到在较长的 DNA 时达到饱和。理论分析与实验中所测得的较短的 DNA 双链分子环化概率的数据一致。概率的数据一致。

关键词：DNA 力学，持续长度

分子马达的力的自我调节

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摘要：在肌肉中存在多个肌球蛋白，是一种分子马达。分子马达在工作时把 ATP 水解所释放的化学能转化为机械能。一个很重要的现象是，虽然单个分子马达的行为本质上是随机的，但多个分子马达的总体行为却是有序的。这种有序性可以提高能量转化的效率。不久前一项清楚地表明在骨骼肌收缩时处于工作状态的分子马达的数目受外力精确调节，并随外力呈线形变化，而单个分子马达上的力基本保持不变。为了理解这一现象，我们建立了首个仔细考虑单个分子马达行为的骨骼肌纤维收缩理论模型，并开发了相应的有限元与 Monte Carlo 方法相耦合的计算方法。基于模型所计算的肌纤维力与收缩速度的关系反演了经典的 Hill 经验公式。我们的工作揭示了单个分子马达独特的力学性能与其特殊的随机特性在调节多个分子马达协调工作中的关键作用。我们进一步在经典的摆动杠杆臂理论的基础上设想当处于工作状态时的单个肌球蛋白的力达到 6pN 左右时，杠杆臂将停止摆动。通过论证，提出杠杆臂停止摆动是由于无机磷酸盐与 ADP 重新结合而产生约束。基于这些假设，建立了单个肌球蛋白的一个机械化学工作循环的动力状态模型。通过分析，获得了在不同收缩速度时处于工作状态的分子马达的力与位移的曲线，与实验中的测量结果一致，证明单个分子马达确实具有独特的弹性力学性能。

关键词：分子马达，　力的调节

内摩擦的动力学起源及其在蛋白质动力学研究中的应用

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摘要:内摩擦问题是蛋白质动力学研究中一个重要而基础的物理问题，得到了多年的持续关注。近年来随着单分子技术的进展，对于分子的内摩擦效应有了更多定量结果，推动了人们关于内摩擦认识，也提出了很多问题，强烈要求从理论上对于内摩擦物理本质的深刻认识。本工作，从一般的郎之万方程出发，利用局部坐标投影的方法，得到了内摩擦的形式。这一形式不依赖于体系序参量的选择，在应用上有很大的普适性，也揭示了其与系统动力学过程及系统能量面之间的内禀联系。利用这一计算形式，针对双阱模型系统，考虑了内摩擦效应后，我们可以得到类似的 Krames 关系，定性解释了实验上内摩擦的线性可加形式。进而，我们针对简化的高分子和蛋白质，分析了内摩擦效应的有关特性，重现了单分子实验中非线性内摩擦形式，还得到了内摩擦对体系大小和温度的依赖关系，其结果和高分子理论对内摩擦物理特性的唯象理论定性一致，并指出了影响内摩擦的物理因素，给出了定量结果，澄清了一些争论。我们还探讨了不同二级结构内摩擦效应的大小，回答了单分子实验提出的一些疑问。通过这一系列研究，我们指出了内摩擦效应是系统动力学的基本特征，并给出了一种定量刻画的方法，对于定量认识蛋白质动力学等物理过程有推动作用。

关键词：内摩擦，蛋白质动力学，郎之万方程，Krames 关系

3-D printing based stent positioning study for PCI prognosis

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Abstract: Percutaneous coronary intervention (PCI) is a widely used and effective treatment for stenotic coronary arteries in coronary heart disease. In PCI, a stent is guided at the bifurcation blockage position, inflated to open the artery and allow blood to flow. However in surgery the physicians are uncertain about optimized stent position in complex geometric coronary landscapes and arbitrary positioning would arouse higher risk for restenosis due to the change of localized flow distribution. In collaboration with Anzhen Hospital, our group designed and constructed a microchip-based in vitro PCI model to study the optimization of the stent position. My talk will present our efforts on introducing the clinic example, constructing the corresponding model with the high resolution 3-D printer, implantation real stent inside the models (in vitro surgery) and analysis for the optimized surgery plan. This work indicates that 3-D printing technology combined Lab-on-Chip idea would have great potentials in medical research and clinic applications.

Key Words：3-D Printing coronary stent, microfluidics

基于水凝胶的微尺度细胞操控技术在生物医学领域的应用

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摘要：随着微纳技术的快速发展，精确操控细胞及细胞-材料“生物转”越来越多的应用于生物力学，组织工程及再生医学等生物医学研究领域。西安交通大学仿生工程与生物力学中心，从生物力学、生物传热学、生物医学等理论体系出发，依托组织工程、细胞打印等相关前沿生物技术，着力于解决生物医学工程的基础性研究以及临床医学治疗方案的设计、优化。本课题组开发出了基于水凝胶材料的微尺度凝胶，并将细胞包裹与微凝胶中在体外培养形成微尺度的细胞-凝胶“生物砖”，再通过磁力，声波，静电力等多种方式将细胞-凝胶“生物砖”精确地组装成不同复杂结构的微组织，用于组织工程和再生医学。本课题还开发了细胞打印技术，该技术是快速成型技术和生物制造技术的有机结合，可实现在三维尺度微米量级上精确控制不同种类的细胞及细胞外基质的分布。利用细胞打印技术，可以高通量地制备包裹于凝胶内的细胞（$>10^2$/s），还可以在微米量级精确控制细胞的位置。载有细胞的水凝胶可以在三维空间上“固定”细胞，且水凝胶高含水量、良好的生物相容性和类自然细胞微环境的性质，利于细胞存活。包裹于凝胶内的细胞可作为细胞传感器的传感单元，故细胞打印技术具备高通量制备细胞传感器传感单元的潜力。因此，利用细胞打印技术可以同时制备成百上千用于药物筛选、疾病检测的样品。

关键词：微纳技术,生物力学，水凝胶，组织工程，组织工程

Role of Serum Proteins in the Initial Attachment of Mammalian Cell

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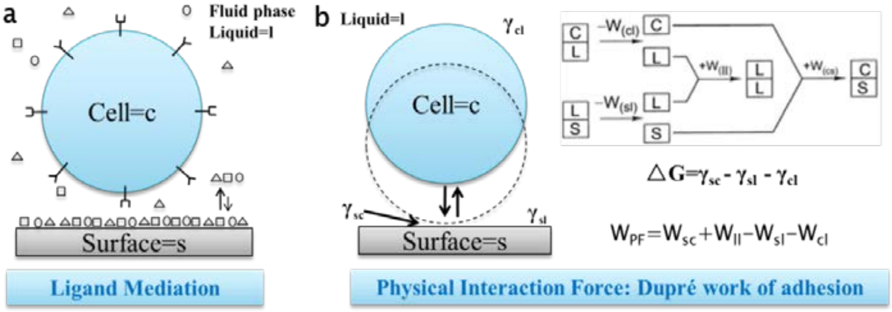
Abstract: Cell adhesion mechanism has been widely explored in the past several decades, however, it is still a mystery as no consensus been reached. The widely accepted biological view suggests that adsorbed proteins on surface mediate cell adhesion. However, The biological theory is untenable at some point as cells could attach without the presence of proteins. We propose that the biologically driven, (ligand-mediated, LM) cell-adhesion process occurs in the ubiquitous context of colloid and interfacial forces (physical interaction forces, PF) that are subsumed into an overall work of adhesion (W_{adh}) equal to the sum of the LM and PF components, such that $W_{adh}=W_{PF}+W_{LM}$. A new "suspension-depletion" method was developed to investigate cell attachment kinetics and further test the hypothesis. Result implies that the W_{PF} term in the above W_{adh} equation dominates short-term cell adhesion, at least until the biology of cell spreading/replication dominates population of the substratum, leading to formation of a confluent monolayer.



Key Words: Cell adhesion, Protein adsorption, Ligand mediation, Physical interaction

Fig.1 Schematic diagram of cell attachment to a surface mediated by biological recognition (a) and physical interaction forces (b). Ligands (such as fibronectin, vitronectin, and fibrinogen) adsorbed from serum-containing medium (represented by circles, squares, and triangles) are thought to undergo specific interactions with cell membrane receptors forming bonds that hold cells to the surface. The physical-force contribution has been formulated in terms of the classical Dupré combination of interfacial energetics.

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FMN核糖开关的动力学调控

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摘要：核糖开关广泛存在于细菌、真菌、植物和动物中，它的发现和 RNA 干扰现象称为近十年（1997-2007）中 RNA 的两个重大发现【1-2】。位于枯草杆菌 ribDEAHT 操纵子的 flavin mononucleotide (FMN)核糖开关是能够与 FMN 特异性结合并引起构象变化，通过调控转录提前终止来调节下游目的基因表达的 RNA 结构元件【3】。对于转录水平调控的核糖开关，其生物功能的实现与转录折叠密切相关。实验发现 FMN 核糖开关的转录终止效率依赖于转录条件【4】，如 RNA 折叠、转录延伸和暂停、代谢物结合等。由于转录过程中构象形成和转换的动态过程无法确定，核糖开关的调控机制以及这些因素对其开关活性的影响也并不清楚。我们发展了能够处理长链转录折叠的 RNA 二级结构宏观动力学方法【5-7】，可以直观的反映 RNA 二级结构转录折叠的行为。采用此方法我们研究了 FMN 核糖开关，给出了在不同条件下（转录速率，暂停，配体浓度）的转录折叠行为。结果表明降低转录速率或者适当的暂停可以延长了转录过程中配体结合的时间窗口，使得更多的 RNA 形成 bound state，从而提高了转录终止效率并抑制下游基因的表达。根据 FMN 核糖开关的转录结果，我们建立了其动力学调控模型，并模拟不同条件下蛋白质生成率。结果显示核糖开关可以通过反馈调节使得周围环境的中配体浓度处于稳定水平，这对生物体的正常运行至关重要。

关键词：FMN 核糖开关，转录折叠，基因调控

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Dimensions of receptor-ligand complex and the optimal radius of endocytosed virus-like particle

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Abstract Recent experiments have pointed out that cellular uptake is strongly dependent on the physical dimensions of endocytosed nanoparticles and the optimal radius of endocytosed virus-like particle coated by transferrin is around 50 nm. As the same time, the dimensions of receptor-ligand complex have strong effects on the size-dependent exclusion of proteins in cell environments. Inspired by these experimental results, a continuum elastic model is constructed to resolve the relationship between the dimensions of receptor-ligand complex and the optimal radius of endocytosed virus-like particle. These results demonstrate that the optimal radius of endocytosed virus-like particle depends on the dimensions of receptor-ligand complex and the dimension of receptor-ligand complex reduces the depletion zone. According to this this model, the density of ligand on the bioparticle also can be deternined and matches with experimental results.

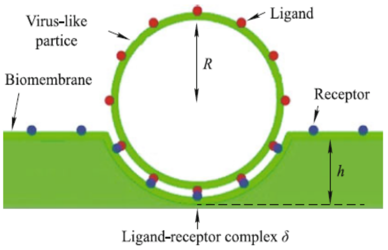

Fig. 1 Representations of endocytosis process of virus-like particle and the effects of dimension of ligand-receptor complex on the depletion effects. The green sphere is the virus-like particle and the green sheet is the biomembrane which includes cytoskeleton.The red and blue solid points represents ligand and receptor, respectively. R, δ and h are the radius of virus-like particle, the dimension of receptor-ligand complex and the engulfment of virus-like particle, respectively.

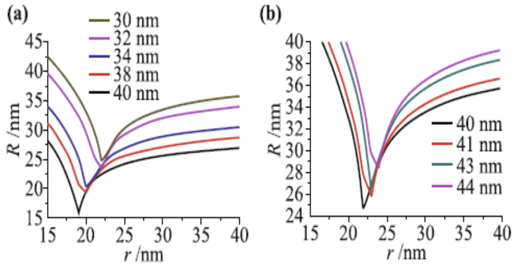

Fig. 3 Contours of dimension of ligand-receptor δ, as a function of R and r, the radii of large particles and small particles, respectively. (a) From bottom to top, dimension of ligand-receptor δ ranges from 30 nm to 40 nm. (b) Dimension of ligand-receptor δ ranges from 40 nm to 44 nm.

Keywords: cellular uptake; depletion effects; dimension of Receptor-ligand complex; elasticity theory

Single Molecular investigation of DNA looping and aggregating by restrictionendonuclease BspMI

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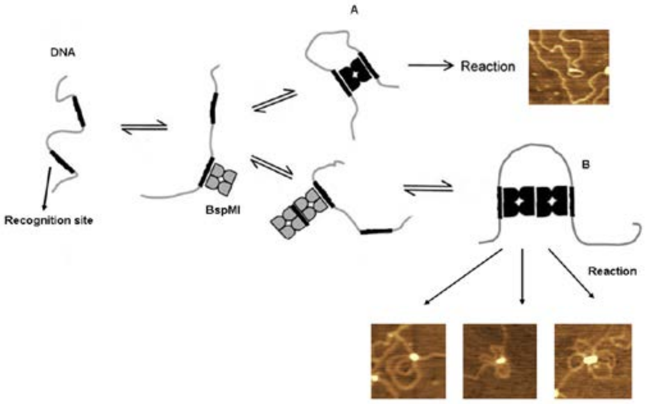
Abstract: DNA looping and aggregating induced by restriction endonuclease BspMI are studied by atomic force microscopy(AFM), magnetic tweezers(MT). Under the condition of substituting Ca2+ for the normal enzyme cofactor Mg2+ and having the enzyme concentration less than the critical concentration of 6 unit/mL, AFM images of DNA-BspMI complex show that the number of binding and looping increases with the enzyme concentration. Through the volume measurement of BspMI-DNA complex, we find that the number of single tetramer BspMI -DNA particle takes over 85% of the complex after 30 min of incubation. At the critical concentration 6 unit/mL, all the BspMI binding sites are saturated, so the loops induced by one tetramer BspMI to bind two sites do not occur. It is worth noting that nonspecific BspMI binding to DNA at saturation concentration represents more than 8% of the total BspMI-DNA complexes in direct visual AFM images, where the number of binding sites is not just 39. Interestingly, we used MT to prove that the additional loops can form when the enzyme concentration is higher than its saturation value (6 unit/mL) and the complex is incubated for a long time (> 2hrs). We ascribe this phenomenon to the aggregation of enzymes. The force spectroscopy of the BspMI-DNA complex shows that the force pulling open the loop of the complex at less than saturation concentration has a peak at about 3pN, which is lower than the force pulling open the additional loops by enzyme aggregated at higher than saturation concentration (>6pN). The statistics of optimum loop sizes about BspMI-DNA complexes were about 900 bp.

Key Words: atomic force microscopy, magnetic tweezers, restriction endonuclease, DNA



蛋白质对低能电子损伤 DNA 的保护机制研究

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摘要:本文首次运用从头计算分子动力学方法，研究了蛋白质对低能电子诱发的DNA损伤的保护机制。文章以典型的非极性氨基酸-甘氨酸（Glycine）与电子吸附性最强的碱基-胸腺嘧啶（Thymine）为例，模拟了低能电子在两者混合物上的局域化过程。 结果显示，蛋白质以两种方式降低了电子对DNA的潜在损伤。如果电子首先被碱基捕获，邻近氨基酸会通过质子转移降低该电子在DNA上的活性，阻碍其进一步反应； 如果相邻氨基酸之间发生了无势垒质子转移，电子则会被氨基酸直接俘获，对DNA发生屏蔽效应，减少DNA损伤的几率。(Phys. Chem. Chem. Phys. 2014 DOI: 10.1039/c4cp03906h.)

关键词：低能电子，DNA损伤，蛋白质，质子转移

DSS1 对蛋白质 PCID2 构象稳定性影响的分子动力学研究

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摘要：固有无序蛋白(IDPs: Intrinsically Disordered Proteins) DSS1 的是主要作用是作为复合体之间的分子粘合剂，在 TREX-2 复合体中的 DSS1 主要与 PCID2 结合，参与转录和 mRNA 的输出之间相耦合的过程。研究发现，DSS1 与 PCID2 蛋白的结合起到了稳定 PCID2 蛋白结构的作用，然而，DSS1 对 PCID2 构象变化影响的动态变化过程的信息尚未可知。为了研究蛋白 DSS1 对 PCID2 构象变化的影响以及 DSS1 与 PCID2 之间的结合机制。我们采用分子动力学（MD）模拟的方法，分别对 PCID2-DSS1 复合体、apo-PCID2 单体以及 apo-DSS1 单体进行了 500ns 的分子动力学模拟。主链碳原子的均方根偏差(RMSD) 、均方根涨落（RMSF）和主成分分析（PCA）表明 bound PCID2 的构象变化小于 apo-PCID2，特别是与 DSS1 结合处的构象(螺旋 Ⅳ和Ⅷ)，二级机构分析表明螺旋Ⅲ 和 Ⅳ 之间的结构与 DSS1 之间形成反平行 β-sheet 的概率升高。我们进一步的采用能量分解的方法计算了 DSS1 残基和 PCID2 残基之间的相互作用能，计算的自由能表明静电相互作用在 PCID2 与 DSS1(42-46)之间的相互作用中起主导作用，而且在 PCID2 与 DSS1 的螺旋区域之间的相互作用中通过七个残基形成了疏水。这些结果与实验得出的结论一致。研究 DSS1 对 PCID2 的作用，可以为深入了解 TREX 复合体在核酸输出中的功能提供帮助。

关键词： PCID2 蛋白，分子动力学模拟，构象变化，结合自由能

Unfolding dynamics of Titin I27 domain studied by magnetic tweezers

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Abstract: Titin, the largest known protein consisting of ~30,000 amino acids, connects Z line to M line in sarcomere and then it limits the contraction/extension range of sarcomere which contributes to passive stiffness of muscle. It is composed by many individually folded domains in the I band, whose unfolding is controlled by force and other molecular interaction, which function as a molecular spring to regulate process of muscular movement. The research on titin has been through a long time but mainly done by using the traditional chemical approach, AFM single molecular manipulation method, and molecular dynamics simulation. The force response behavior of titin has been systematically researched by AFM single molecular manipulation which focus on the force range above 100 pN because of its technology limits in small force region.Unfolding process of titin under physiological force range of <100 pN is still vague.

In this report, we studied the unfolding process of titin I27 domain in physiological force range of 6-110 pN, by using home-made improved magnetic tweezers. Our home-made magnetic tweezers makes it possible to study a single protein for multiple hours with improved force resolution and large force range. We found that in the force region from 6 to ~25 pN, the unfolding time increases with increasing force, i.e., larger force makes I27 more difficult to unfold in this force range. This phenomenon is opposite to physical intuition and also against the prediction from AFM single molecular experiment data, and challenge classic views of protein unfolding dynamics

Key Words: titin, I27, protein unfolding, magnetic tweezers

应用单分子 FRET 技术观测蛋白质折叠

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摘要：包括 FRET 在内的单分子技术能够彻底避免传统测量技术的系综平均，进而观测单个分子的状态以及单个分子在不同状态之间转化，所以单分子技术是研究生物大分子结构和相互作用的有力工具。但是荧光分子发光效率普遍会受到光物理和光化学过程的影响，而低下的发光效率会严重限制单分子 FRET 的时间分辨率和在生物学研究的应用，我们发展了一种新型荧光保护方法将单分子 FRET 技术的时间分辨率提高一个数量级，达到 10 微秒级。

经典的蛋白质折叠两态模型认为蛋白分子在折叠过程中会出现两个构象群体，而单态无能垒折叠理论（downhill folding）则认为：某些单态无能垒蛋白可以仅有一个构象群体。但由于原有的单分子 FRET 技术时间分辨率太慢不能测量快速折叠蛋白的构象分布，所以单态无能垒蛋白的存在性引起了很大的学术争议。我们应用快速 FRET 技术首次观测到了单态蛋白 BBL 在折叠过程中所出现的单群体构象分布，证实了单态蛋白的存在。

另外在两态蛋白研究中，我们应用单分子 FRET 技术发现两态蛋白 SH3 的两个构象群体的分子构象在折叠过程中都有显著的变化，并非如两态模型所认为的静止不变或变化很小，这一结果和上述的单态蛋白实验都表明传统的两态模型过于简化，忽略了很多蛋白质折叠的重要特征，所以我们应该在能量绘景（energy landscape）理论的基础上，建立能够解释在折叠过程中蛋白质构象变化的新的蛋白质折叠模型。

神经元对突触输入信号整合的双线性法则

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摘要：神经元是大脑处理信息的最基本的单元，它是由树突、胞体和轴突这三部分构成，其中树突是接收上游神经元传递过来的电信号并对这些信号进行整合，从而激起胞体处的膜电位的改变，目前很多实验表明神经元的树突对于信号的整合过程是一个非线性过程，但是实验和理论上一直缺乏对于整合过程的精确定量的描述，我们从理想的模型出发，考虑一对突触输入的情况，利用渐进分析的方法得到了关于树突整合过程的解析定量的刻画，一对输入激起的胞体处的电压 VS 反应等于单个输入激起的胞体处的电压反应(V1 和 V2)的和，再加上某个分流系数 k 与 V1 和 V2 乘积的双线性项。正是由于该双线性项的存在，我们将该法则定义为双线性求和法则，令人惊讶的是，尽管这个双线性法则是基于理想模型得到的，但是我们进一步的神经元的数值仿真模拟以及电生理实验，都验证了该双线性法则的适用性，我们的结果表明：神经元对于多个突触输入的整合效应可以分解为所有可能的每两对突触的输入的效应的和，其中任意两对突触的输入效应服从相应的双线性法则。

Bilinearity in spatiotemporal integration of synaptic inputs

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Abstract:A neuron receives thousands of synaptic inputs from its dendrite and integrate them to process information. Many experimental results demonstrate the dendritic integration could be highly nonlinear, yet few theoretical analysis has been performed to obtain a precise quantitative characterization analytically. Based on asymptotic analysis of a passive cable model, we derive a bilinear spatiotemporal dendritic integration rule for a pair of time-dependent synaptic inputs. Surprisingly, the above rule, which is obtained from idealized models, can be verified both in simulations of a realistic pyramidal neuron model and in electrophysiological experiments of rat hippocampal CA1 neurons. Our results demonstrate that the integration of multiple synaptic inputs can be decomposed into the sum of all possible pairwise integration with each paired integration obeying a bilinear rule.

The origin of drop splashing – a wind ten times stronger

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Abstract: When a fast-moving drop impacts onto a smooth substrate, splashing will be produced at the edge of the expanding liquid sheet. This ubiquitous phenomenon lacks a fundamental understanding. With high speed photography, we illustrate that the ultra-thin air film trapped under the expanding liquid front triggers splashing. Because this film is thinner than the mean free path of air molecules, the interior air flow transfers momentum with an unusually high velocity comparable to the speed of sound, and generates a stress ten times stronger than the general situation. Such a 'strong wind' initiates Kelvin-Helmholtz instabilities at small length scales and effectively produces splashing. Our model agrees quantitatively with experimental verifications, and brings a fundamental understanding to the ubiquitous phenomenon of drop splashing on smooth surfaces.

Key Words: drop splashing, Kelvin-Helmholtz instability, wetting

Structural origin of fractional Stokes-Einstein relation in glass-forming liquids

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Abstract: The Stokes-Einstein relation has long been regarded as one of the hallmarks of transport in liquids. In many glass-forming liquids, Fractional Stokes-Einstein relation (SER) is observed after the breakdown of SER above glass transition. Using molecular dynamics, we investigate the dynamic properties in glass-forming liquids. We find that SER breaks down when the size of the largest cluster consisting of trapped atoms starts to increase sharply at which the largest cluster spans half of the simulations box along one direction, and the fractional SER starts to follows when the largest cluster percolates the entire system and forms stable 3-dimentional network structures. Further analysis based on the percolation theory also confirms that percolation occurs at the onset of the fractional SER. Our results directly link the breakdown of the SER with structure inhomogeneity and onset of the fraction SER with percolation of largest clusters, thus provide a possible picture for the breakdown of SER and onset of fractional SER in glass-forming liquids, which is important for the understanding of dynamic properties in glass-forming liquids.

Key Words: Glass transition, Stokes-Einstein relation, percolation dynamic crossover

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Theory of glassy dynamics in the system of model colloidal chains

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Abstract: Slow dynamics and the glass transition have long been the subjects of intensive study in condensed matter physics. Colloids are an excellent model systems which have been investigated extensively by experiments, simulations and theories. Nonlinear Langevin equation (NLE) theory is one of the microscopic theories of glassy dynamics which has been applied to study the relaxation, elasticity, aging and mechanical responses in both colloidal and polymer glasses. This theory is built on the system of particles. And, it was extended to polymeric systems with chain-like structures by simply replacing the correlation function and structure factor of particles or colloids by those of polymers. In this work, we modified the NLE theory to include the effect of intra-chain correlations in a consistent way. The vertex of the integral in the expression of dynamic free energy splits into two terms, both of which are explicitly depend on the intra-chain correlation function. We applied the theory to study the glassy dynamics of model colloidal chain system and compared the result with the pure colloidal glass. In the model, we adopt the approximate Koyama distribution for worm-like chain to account for the strong excluded volume interaction between colloids along the same chain. We found the crossover volume fraction Φ_c increases with N, the number of colloids in the chain, and saturates at large N, but deceases with bond length and rigidty. The localization length at the crossover, R_c which is related to the Lindeman length is not very sensitive to N. It decreases from 0.19σ to 0.165σ when N increases from 1 to 100. But, R_c increases slightly with bond length and rigidty. The localization length and the relaxation time both increase as the rigidity of the chain becomes larger which is in consistent with the predictions of Mode Coupling Theory on the glassy behavior of chain-like molecules. We found the glass transition volume fraction increases with chain length, but decreases with bond length and rigidty.

Key Words: glass, colloid, colloidal chain, intra-chain correlation function

Dynamic structures in dry active fluids

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Abstract: Active matter, which is a physical abstraction of running animals, flying birds, marching locusts, swimming bacteria, migrating cell or even cytoskeleton, has been a new building block for physicists over the last decade or so to understand the common collective behavior in these non-equilibrium systems. The liquid crystal state of active matter is of particular interesting since the collective dynamics is coupled with large scale liquid crystal order. Dynamic instabilities are widely observed in active liquid crystal systems. This often leads to large-scale collective motion in active nematics. Here we would like to present interesting dynamical properties of two model active nematic systems when instabilities take place.[1-2] In a toy active nematic system where the interaction only tends to align intersecting needle particles, we predict long-wave length instabilities and further show large-scale chaotic evolution in such system. We also use hard elliptic rods instead of penetrable toy needles to simulate active nematic state. We find the instability in deep nematic order is characterized by the active unbinding of topological defects. These defects behave very differently to non-active systems. We further reveal that their anomalous dynamics may lead to large-scale collective motions in such active granular system

Key Words: active matter, active nematics, topological defects, dynamic instability, hydrodynamics

Reference:

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水溶液中冰的均质行核

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摘要：水的晶化是自然界最为普遍的液固转变之一。冰晶核的形成和长大在该过程中扮演着重要的角色。根据有无外来介质作为行核质点，行核过程可分为异质行核和均质行核。冰均质行核过程直接影响大气对流层顶端卷云的性质，进而影响整个地球的气候。 自然界条件下冰的均质行核多是在有溶质参与下完成的。由于模拟和实验上的困难，对水溶液中冰的均质行核过程的研究并不充分。

最近，我们成功地发展了一个方法，来确定晶化后水溶液中初生冰相的含量。该方法的重要性在于：对于大多数水溶液，即使以较慢的速度冷却，在初生冰相析出后，剩余浓缩相会发生非晶化。在确定非晶化浓缩相浓度方面，我们发展的方法比目前常用的方法更准确。如果把初生冰相对应的水分子定义为自由水，而发生玻璃化的水分子定义为结合水，我们发现不同浓度的不同类型水溶液在相同自由水含量条件下具有相同的冰均质行核温度、初生冰相的熔化温度。我们同时建立了自由水含量与过冷水溶液活度的关系，讨论了深过冷水热力学性质与温度的关系。依据自由水的量分别与活度、均质行核温度间关系，讨论了表征水溶液中冰均质行核的活度理论和目前普遍支持的 two-step model 间的关系。

关键词：均质行核, 水溶液，自由水和结合水，活度

A novel method to create fast growing biofilm

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Abstract: Biofilm is a group of cells bounded by extracellular polymeric substance (EPS), growing on wet environment, usually on surfaces. It can survive in extreme conditions and is responsible for over 80% of microorganism infections in human [Ref. 1]. However, the research on biofilm is hindered by the slow formation of biofilm in laboratory, especially for *E. coli*, the most understood bacteria. For *B. Subtilis*, a typical biofilm-forming strain, it usually took 48 to 72 hours for biofilm to form using traditional method [Ref. 2-5]. For *E. coli*, it took even longer: it took weeks to produce ~ 10-100 μm^3 of biofilm by traditional *E. coli* biofilm reactor[Ref. 6-9]. In order to have higher yields, people tried to use different methods to cultivate biofilm: such as repeating the dipping-drying process in the traditional method to increase the number of cells at the beginning of the growth, or, using the glass-wool reactor, which is using the increased surface area to get more yield. These methods may double or triple the yield, but the amount is still in the range of ~ 100μm^3 after weeks of waiting. By using a novel method to encapsulate bacteria, for both *E. coli* and *B. Subtilis* strains, ultra high cell volume fraction was reached at about 1000 times more than saturated culture, and the biofilm formation rate increased at least two orders of magnitude. High density is one of the key strategies of bacteria surviving in stressed environment [Ref. 10]. The cell volume fraction in this method can reach above 63%, the critical density limit for motile cells to form clusters called "living liquid crystal" [Ref. 11, 12], this number is 1000 times larger than that of the saturated culture -- highest cell density under traditional conditions. Motility of cells was monitored and characterized before biofilm formation. Possible mechanism for this fast biofilm formation was discussed and further studies were also suggested. The mechanism of this fast growing process may lead to significant discoveries in life sciences, because many organelles in nature such as alveoli and renal tubule have similar features geometrically and structurally.

This novel method not only made it possible for *E. coli* to be used as a model strain to study biofilm, but also drove us to explore unknowns towards the essential mechanism and formation conditions of biofilm.

Key Words: Biofilm, microfuidics, bacterial motility, biophysics

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软物质液滴蒸发/干燥过程中空腔形成基理

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摘要：在软物质（高分子、胶体）溶液蒸发或干燥过程中，人们会经常发现空腔或气泡等的产生。这类软物质常见于我们的日常生活中，如咖啡，牛奶等。通过喷射蒸发/干燥软物质液滴制造纳米或是微米级空心球广泛存在于大量工业应用中（食物、药物、功能性颗粒制造等）。我们在这个工作里用一个简单的模型描述复杂的空心球形成现象。通常在这类软物质溶液蒸发过程中会在溶液表层形成一层具有黏弹性的表面层，而在软物质溶液中非常多的不稳定现象（如空腔/气泡产生，皱纹形成、液滴塌缩等）都和这皮肤层有关。我们在这里很好的解释了空腔的形成是由于在蒸发过程中形成的皮肤层的弹性能和空腔的表面能相互竞争的结果。同时，我们给出空腔形成的条件，包括内外压差、表面张力、皮肤弹性等。所得到的结论和现有的实验有很好的符合，这是对于空腔产生的物理原理的简单阐释，也可能为将来工业应用能有很好的指导意义。 同时，这过程非常复杂，我们忽略了动力学在过程中的作用（如皮肤层的产生，气泡成核等），所以需要大量工作来理解这复杂的过程。在接下来的工作里，我们将过程中动力学进行一定程度的探索。

关键词：软物质液滴、蒸发/干燥、空腔

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Cavity formation in drying droplets of soft matter solutions

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Abstract： When a droplet of a soft matter solution is dried, cavities are often formed in the droplet, giving a hollow sphere in the end. A theoretical model is given for this phenomenon. It is shown that the formation of a gel like layer (skin layer), which has a finite shear modulus, is essential for the phenomenon to take place. The condition for cavity formation (how it depends on the shear modulus and thickness of the skin layer), and the variation of the droplet volume and cavity volume after the cavity formation are examined. However, there still exist lots of unsolved problems, among which dynamical part is very important. So next step we will look at the dynamical process, and want to find interesting explanation for this complex phenomenon.

单羟基醇氧族衍生物在玻璃转变区间内的动力学研究

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摘要：由于氢键在生物生存中的重要性，对氢键液体的研究一直是个热门课题。单羟基醇是一类典型氢键液体，然而不同于大多数物质，该类物质处于过冷态时的介电弛豫谱中常在低频处观察到一个“额外的”德拜型弛豫[1]，伴随在高频侧出现另一个弛豫。研究发现：高频处的弛豫对应真正的结构弛豫，与粘度与玻璃转变相关[2,3]。实验证实，单羟基醇中的德拜弛豫与氢键所引起的结构密切相关[4]，但是与德拜弛豫对应的氢键结构的微观模型与物理起源依然还没定论。可以预见，单羟基醇中的德拜弛豫一定与分子结构相关，通过改变单羟基醇分子的结构来分析介电弛豫动力学的变化，将会有助于理解德拜弛豫的物理起源。我们利用介电技术开展了该类物质过冷液体的弛豫动力学研究，发现对于用一个硫原子替代单羟基醇分子中碳原子而形成的 3-甲硫基-1-己醇，德拜弛豫不会被破坏[5]。进而我们选择用一个氧原子替代单羟基醇分子中的碳原子而形成的氧基醇，表观上在介电谱上只观察到一个主弛豫，然而通过系统分析，我们发现所有这些液体的主弛豫的半高宽随温度的增加出现了最小值，即随温度先变窄而又加宽，不同于常规液体的结构弛豫宽度的时温叠加原理或者随温度升高而变窄的行为。进一步研究发现，基于该弛豫半高宽而得到的非指数性因子β_{KWW}，不遵循常规液体β值介电弛豫与焓弛豫测量一致性原则，也不满足非指数性因子与液体强弱性因子 m 之间的 Böhmer 关联。该研究为深入理解氢键动力学提供了实验依据。

关键词：玻璃转变, 介电弛豫， 德拜弛豫， 单羟基醇

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From Crystals to Disordered Crystals: A Hidden Order-Disorder Transition

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Abstract: Order and disorder constitute two fundamental themes in condensed matter physics and material science. An integrated understanding of materials ranging from crystals to disordered solids requires organizing principles from both sides, and in between. Perfect crystals, the epitome of order, provide an important starting point for understanding properties of solids, which lie in the heart of solid state physics. In contrast, materials such as glasses and granular assemblies are highly disordered. Although the absence of long-range structural order makes it difficult to achieve analytical descriptions, disordered solids have been shown to exhibit a set of universal properties distinct from their crystalline counterparts, e.g., the excess low-frequency excitations and subsequent thermal anomalies, the heterogeneous mechanical response to perturbations, and the dynamic heterogeneity through the glass transition. While much attention has focused on the peculiar properties of disordered solid itself, there has been comparatively little research into the crossover between the crystals and disordered solids, leaving the boundary between the two extremes of order and disorder elusive.

In this study, we perform detailed investigations into the evolution from perfect crystals to disordered solids, by using particle-size polydispersity as the control parameter. Within similar framework, previous simulations have shown that the system undergoes structural amorphisation toward an amorphous solid state when the polydispersity increases over a sufficiently large value. Here we report a hidden order-disorder transition from crystals to disordered crystals, namely solids with extremely high crystalline order but mechanical properties resembling typical amorphous solids, long before the structural amorphisation. With the bond orientational order and translational order insensitive to this transition, multiple mechanical properties show a sudden change. The evolution of the underlying mechanical network plays a key role in characterizing the hidden order-disorder transition, which is controlled by the volume fraction with respect to the close packing point and the particle-size polydispersity. We construct a phase diagram which provides a unified view of solids between the mechanical extremes of order and disorder. Moreover, scaling analyses performed in disordered-crystal regime reveal new jamming physics, the study of which may deepen our understanding of disordered solids.

Key Words: crystal, disordered crystal, order-disorder transition

Speciation in Aqueous Magnesium Polyborate Solutions at 298.15K

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Abstract Density, conductivity, viscosity, and pH of $2MgO:3B_2O_3$ (for inderite, $2MgO\cdot 3B_2O_3\cdot 15H_2O$), $MgO:7B_2O_3$ (for hungchaoite, $MgO\cdot 2B_2O_3\cdot 9H_2O$) and $MgO:10B_2O_3$ (for mcallisterite, $MgO\cdot 3B_2O_3\cdot 7.5H_2O$) solutions have been measured during isothermal evaporation at 298 K. A complete set of thermodynamic equilibrium constants of magnesium borates were obtained on the basis of the basic principles of thermodynamics. The species distributions were calculated by Newton iteration method with pH and thermodynamic equilibrium constants, as shown in Fig 1. The main species in aqueous $MgO:1.5B_2O_3$, $MgO:7B_2O_3$ and $MgO:10B_2O_3$ solutions were verified by Raman spectra, as shown in Fig 2. The main species in $2MgO:3B_2O_3$ solution is $B_3O_3(OH)_5^{2-}$, in step with the congruent inderite. Here, It is interesting to note that the dominant species in aqueous $MgO:7B_2O_3$ solution is not $B_4O_5(OH)_4^{2-}$ in hungchaoite solid, but $B_3O_3(OH)_5^{2-}$, agrement with the incongruent hungchaoite. More interestingly, the dominant species in aqueous $MgO:10B_2O_3$ solution is neither $B_6O_7(OH)_6^{2-}$ in mcallisterite solid nor $B_4O_5(OH)_4^{2-}$ in hungchaoite solid, but $B_3O_3(OH)_5^{2-}$, in accord with the incongruent hungchaoite. Compared with the polyborate solutions of Li^+, Na^+ and K^+, the hydration affinity, octahedral structure and configuration of bivalent Mg^{2+} strongly affected the solvent tetrahedral structure first of all, further changed the structure of polyborates. Such a solution environment not only inhibited the hydrolysis of polymers at lower concentration and the polycondensation of oligomers at higher concentration.

Keywords: Polyborate;Speciation;Hydrolysis;Polycondensation

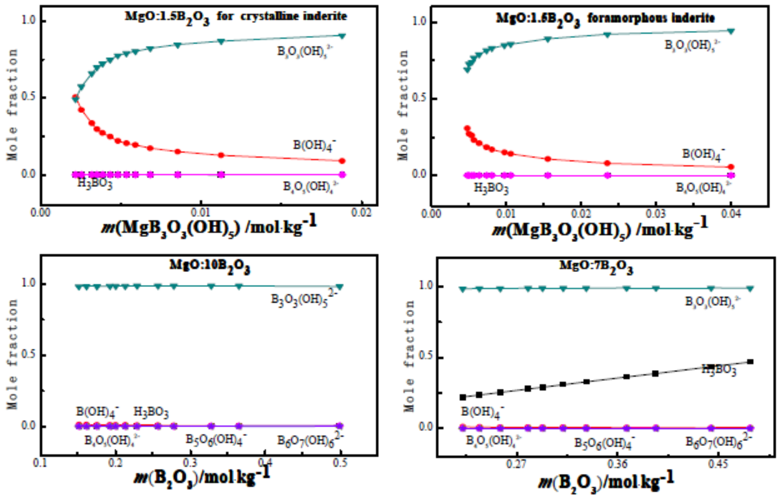

Fig. 1 Polyborate distribution in $MgO:1.5B_2O_3$, $MgO:10B_2O_3$ and $MgO:7B_2O_3$ solutions

■,H_3BO_3; ●,$B(OH)_4^-$; ▲,$B_3O_3(OH)_4^-$; ▶,$B_3O_3(OH)_5^{2-}$;♦,$B_4O_5(OH)_4^{2-}$; ◀,$B_5O_6(OH)_4^-$;★,$B_6O_7(OH)_6^{2-}$

冰熔化的尺寸效应

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摘要：熔化是自然界中常见的从固态到液态的相变。对于水而言，由于其在材料科学、生物学、地质学、农学、气象学等领域的重要性，长期以来人们对冰的熔化及其尺寸效应有着特别的兴趣。目前，对于冰的熔化及其尺寸效应的研究，一方面文献中的数据之间存在着较大差异；另一方面，样品尺寸对熔化的影响机理还很不清楚。尤其是一直以来，人们对于纳米尺度冰熔点的降低量 ΔT 与样品尺寸的倒数 1/d 之间，究竟是线性关系、还是非线性关系，还无法达成共识。

近年来，随着有序介孔材料如 MCM-41 和 SBA-15 的发现，为冰的熔化研究提供了新的选择。本文制备了一系列孔径在 1.7 nm - 11.5 nm 之间、不同孔径的介孔 SBA-15 样品，研究冰熔化的尺寸效应。介孔的孔径用 N_2 吸附法进行表征，介孔中冰的熔点和熔化焓用低温差示扫描量热仪进行测定。

所得结果表明，介孔氧化硅中冰熔点的降低 ΔT 与孔径倒数 1/d 呈线性关系。进一步的分析表明，近年来文献所报道的 ΔT 与 1/d 之间的非线性关系，主要起源于在利用 N_2 吸附法表征孔径时，所利用的吸附回线的吸附分支，与脱附分支相比，所得孔径较真实孔径偏大。即是说，所观察到的 ΔT 与 1/d 之间的非线性关系应该是一个数据分析带来的假象。

熔化焓的数据支持 S. L. Lai 等人的两相模型，即完全忽略表面类液层对熔化焓的贡献。

关键词：水，晶体熔化，尺寸效应，熔化焓

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水表面张力虚部的实验测定

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摘要：我们应用复模量、复介电常数和复磁导率描述材料的力学、介电和磁的动态响应，它们的虚部表征了材料的能量耗散速率，而且虚部与实部具有内在的相互联系；然而，传统上对于液体的表面，我们仅仅用实数表示的表面张力系数来表征液体表面的动态力学响应行为。最近我们提出：液体的表面张力系数应该用复数表示，也就是说，液体的表面也会耗散能量，因此需要用复数来描述液体表面的动态力学响应行为。本报告提出三种完全不同的实验方案：1）表面波的光散射法；2）表面波的共振吸收力学谱；3）液体弯月面的动态响应法（利用基于原子力显微镜的微流变仪）测量了水的复表面张力系数，得到一致的实验结果，这些结果表明：液体的表面张力系数数应该用复数，而不是简单地用一实数表示。

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Metastable Phenomenon in Aqueous Lithium Tetraborate Solutions

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Abstract The metastable phenomenon of aqueous $Li_2B_4O_7$ solution has been observed at 298 and 323K by isothermal evaporation. It is interesting that the maximal supersaturation $[w-w_0)/w_0]$ even reached 12 times. A sticky colloidal soft matter was obtained in the final stages of evaporation. Precipitated solid, sometimes is amorphous without any Bragg peak, sometimes is the crystal with Bragg peaks. The density, conductivity and pH of the supersaturated solutions at the different evaporation stage have been tracked and measured at 298.15 and 323.15 K, respectively. The species distributions were calculated by Newton iteration method from pH and the chemical stoichiometricequilibrium constants of borates[1]. Among them, the dominant species in the supersaturated solution at 298.15K is cyclic chained anion $[B_4O_6(OH)_2]_n^{2n-}$, the minor species isolated anions $B_3O_3(OH)_5^{2-}$, $B_3O_3(OH)_4^-$ and $B(OH)_3$, and the negligible species $B_5O_6(OH)_4^-$ and $B(OH)_4^-$; while the dominant species at 323.15K is still $[B_4O_6(OH)_2]_n^{2n-}$, the minor species $B_3O_3(OH)_4^-$ and $B(OH)_3$, and the negligible species $B_3O_3(OH)_5^{2-}$, $B_5O_6(OH)_4^-$ and $B(OH)_4^-$. The lithium tetraborate trihydrate $Li_2B_4O_7{\cdot}3H_2O$ is the most stable congruent compound in the ternary system Li_2O-B_2O_3-H_2O phase diagrams[2] at 283-353K, having the structural formula $Li[B_2O_3(OH)]{\cdot}H_2O$[3] or $Li_2[B_4O_6(OH)_2]{\cdot}2H_2O$. According to the chemical species distribution, the inter-conversion rules among all the borate anions and their variation rules with temperature in the metastable aqueous solutions have been summarized in the present paper, and the origin of the metastable phenomenon of $Li_2B_4O_7$-H_2O system revealed also.

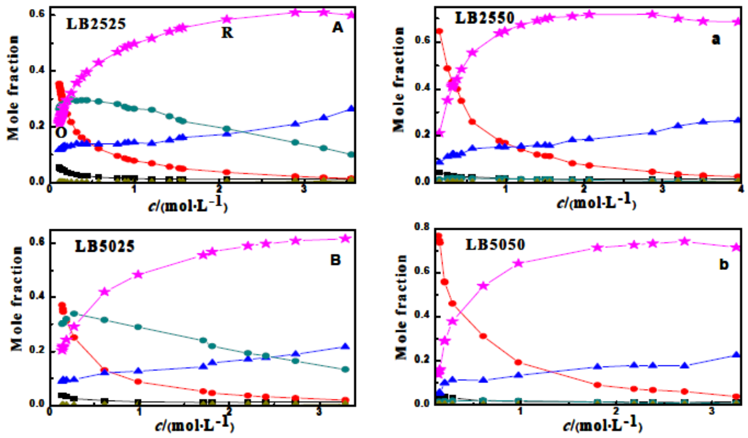

Fig. 1 The chemical species distribution of supersaturated $Li_2B_4O_7$e solutions at 298.15 and 323.15 K

● $B(OH)_3$, ■ $B(OH)_4^-$,▲ $B_3O_3(OH)_4^-$,★ $B_4O_6(OH)_2^{2-}$, ● $B_3O_3(OH)_5^{2-}$,▲ $B_5O_6(OH)_4^-$

超声场中液滴的动态行为研究

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摘要：利用超声悬浮技术将液滴(10μL)稳定悬浮于空气中，并通过声辐射压控制液滴的变形率。关闭声悬浮电源，压扁液滴在重力作用下做自由落体运动。本文采用高速摄影技术研究了压扁液滴自由落体过程中的形态演变。实验中利用表面活性剂十二烷基硫酸钠(SDS)对液滴性质进行调控，系统研究了不同浓度液滴在不同变形率条件下的动态行为，实验发现，液滴的形态演变显著依赖于 SDS 浓度和液滴的变形率。图 1 给出了不同液滴的形态演变过程和相图。 有趣的是，SDS 浓度为 0.8cmc 时，液滴可较长时间保持压扁形态而不回复成球形。经受力分析，界面的 Gibbs 弹性不足以完全抵消 Laplace 压差所产生回复力。声场作用下产生的宏观表面浓度梯度导致强烈的 Marangoni 效应，赋予界面以额外弹性，从而与液滴回复力相抗衡。

关键词：液滴，表面张力, Marangoni 效应，界面黏弹性

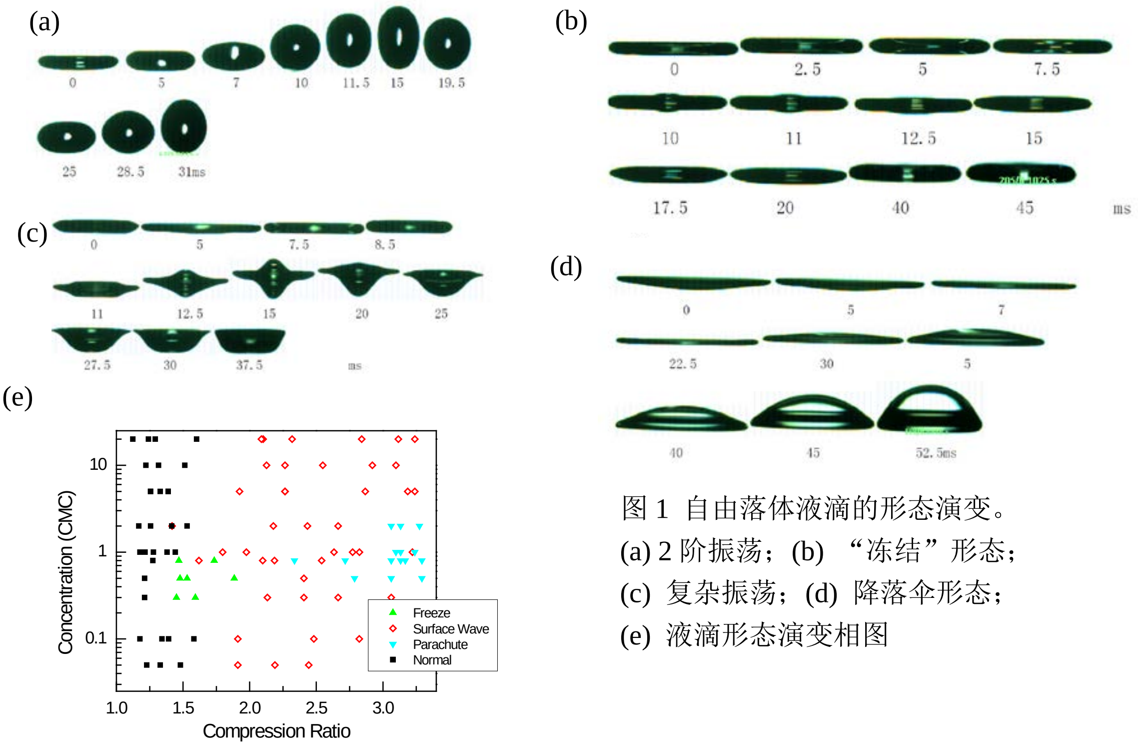

图 1 自由落体液滴的形态演变。
(a) 2 阶振荡；(b) “冻结”形态；
(c) 复杂振荡；(d) 降落伞形态；
(e) 液滴形态演变相图

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分子液体 1-Methylindole 的 JG-β 弛豫动力学研究

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摘要：玻璃转变是一个复杂的动力学微观不均匀过程，宽频介电技术是研究过冷液体弛豫动力学的重要手段。α 弛豫是玻璃转变过程中的最主要的弛豫行为，在玻璃转变过程中广泛存在，是体系中的较大尺度区域的协同运动[1]，在玻璃转变过程中起着主要作用。研究也发现 JG-β 弛豫也与玻璃转变及玻璃态稳定性密切相关[2]。相比于结构弛豫，对 β 弛豫的认识还存在争议，对小分子纯物质的研究通常认为该弛豫是玻璃态中整个分子在小范围内的局域运动[3]，但是对于刚性较弱的分子在外界激励下（如交变电场）其结构内部可能存在某个极性集团的转动，从而产生比 JG-β 弛豫更快的 γ 弛豫，对 JG-β 弛豫的认知产生非常大的干扰。Blochowicz 在二元混合和 Capaccioli 高压方面的研究表明 JG-β 弛豫的广泛性[4,5]，更多的证据仍被期望证实该动力学的普遍性。我们通过综合考虑分子刚性[6]、极性、氢键的影响以及玻璃形成能力等因素，选择具有刚性高、中等极性且无氢键的 1-Methylindole 进行了介电弛豫研究，发现除了主弛豫（α 弛豫）以外，出现了明显的二级弛豫，对该动力学的系统分析表明该弛豫为 JG-β 弛豫。研究结果表明 JG-β 弛豫与氢键诱发团簇无关，进一步证明了 JG-β 弛豫在小分子液体中的普遍性，为 JG-β 弛豫的深入研究提供参考。

关键词：玻璃转变，弛豫动力学，JG-β 弛豫

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基于时序模型法分析光阱中粒子布朗运动

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摘要：光阱中粒子的布朗运动，是光阱中粒子和液体及激光的相互作用的结果，通过对光阱中粒子的运动分析，可以得到粒子、液体以及激光的特性参数。这里，我们采用时间序列分析法对光阱中粒子的运动建立随机模型，进而研究光阱刚度标定及消除光镊随机漂移的方法。

基于建立的模型，我们通过计算其现代功率谱，进而实现对光阱刚度的标定。这种方法可以实现短数据精确标定，这将降低数据采集时间，从而有可能实现光阱刚度的实时标定。为了研究这种方法的有效性，我们采用仿真和实验两种方法，研究了光阱刚度标定结果和数据长度的关系，以及两种方法研究不同捕获深度同光阱刚度的关系，研究结果表明，我们所研究的方法比传统的功率谱法标定结果精度更高。该方法有可能在化学、生物等只能获得较少数据的情况下实现光阱刚度的标定。

同时，基于建立的模型，我们还采用卡尔曼滤波的方法对光镊系统的漂移进行了滤波研究。对实验室的设备研究结果表明，采用该方法有效的降低了光镊系统的随机漂移误差。 本工作得到自然科学基金（Nos. 11302220、11374292）资助。

关键词：光镊，时间序列模型，光阱刚度，卡尔曼滤波

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Reconstructing equilibrium distribution of complex systems use RWED method

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Abstract: Molecular dynamics and Monte Carlo simulation methods had a very deep influence on materials science, biology, and many other fields. Despite their great success, the simulation methods suffer from limitations in quasi-ergodicity in complex systems such as biological macromolecules, thus reduce the scope of their applications. To more sufficient explore the complex conformational spaces, various advanced simulation methods had been developed and applied widely. By using multiple simulation trajectories, which started from dispersively selected initial conformations, the reweighted ensemble dynamics method (RWED) is designed to robustly and systematically explore the hierarchical structure of complex conformational space through mapping trajectories into some selected basis functions then doing spectral analysis of the variance-covariance matrix of the trajectory-mapped vectors (1). However, in RWED, the selection of basis functions is not straightforward. In previous study, we chose the basis functions by physical intuition. But, in more complex cases, it is not trivial task. It is necessary to develop more general method to choose basis functions. In this paper, we focus on the question of choosing generally basis functions for RWED analysis, and present three approaches.

I: Many various analytical physical quantities, such as dihedral angles, radius of gyration, distances of atom pairs, solvated energy, and helix probability, could be applied as basis functions.

II: Cell functions in the space spanned by the physical quantities. We split the physical quantity spanned space into some discrete cells, and define cell functions as basis functions in RWED.

III: RMSD-based-Cell functions. With a similar technique to Markov State Models (2), but different spirit, we develop a method to select basis functions for RWED. Based on RMSD (root mean square deviation) between conformations, we can split sampled conformations into overlapped cells. Those cells were analyzed by PCA (principle component analysis) to get a set of orthogonal basis functions for RWED analysis.

We employ those approaches to analysis three different model systems, two dimensional multiple-well toy model, lattice spin model (2D 8-state Potts model), and a short peptide with implicit solvent, to assess the performance of RWED. In all those systems, starting from different biased initial distributions, RWED could reconstructed equilibrium distribution of them, suggesting the robustness of RWED and the selection methods of basis functions.

Key Words: Free energy surface, RWED, Basis functions

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增强构象抽样的广义正则系综温度空间行走方法

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摘要：增强抽样理论与方法用于提高分子模拟的有效性，然而面临相变存在和势能面复杂对象系统，如蛋白质和生物膜等生物大分子时，现有常规方法的有效性受到很大影响。我们基于广义系综分子模拟的思想，发展了一种在温度β(=1/kT)空间中随机行走的增强抽样方法，它区别常规的能量 E 空间随机行走。该模拟方法在构建的二维(β,E)空间中，使用 Langevin 随机运动方式控制宏观β上的“慢运动”，而在微观层执行广义正则系综下的 Monte Carlo 或分子动力学行走（相对而称“快运动”）。该思想可以看作是模拟回火方法的连续化形式；其中关键在于引入的广义正则系综形式，它能约束构象的势能分布为单峰稳态型，从而能够克服相变或亚稳态降低有效构象抽样的问题。我们给出了该研究的问题背景和基本理论，然后在二维 Potts 模型和 Lennard-Jones 粒子系统中，基于 Monte Carlo 模拟和分子动力学模拟的数值结果，进行了增强抽样的性能分析。对比常规正则系综下的数据结果显示，采用广义正则系综的处理能够加快模拟的各态历经性，显著增强了模拟结果的收敛速度。另外也将该方法改进为自适应方式，用于探测生物蛋白系统的构象折叠。

关键词：广义系综，模拟回火，增强抽样, 构象折叠

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Energy dissipation and adaptation accuracy

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Abstract: As a paradigmatic example of environmental monitoring in biology, the E.coli chemotaxis has been a model system to study cellular response to environmental change. The great signal sensi- tivity and the ability to adapt over a large range of external ligand concentration have attracted much attention and thus have been intensively studied. The energetic cost for maintaining high adaptation accuracy is addressed recently by Lan et.al. and they propose that energy is dissipated to achieve better adaptation accuracy. Based on systematic analytical and computational study on the sensory network model proposed by Lan et.al., deep understanding of adaptation error is achieved in microscopic system. The total energy dissipation is decomposed into the heat dissipated by methylation process and activity switch respectively, which shares a deep connection with the corresponding violation of Fluctuation-Dissipation Relation(FDR), inspired by the FDR-Sasa equality. The adaptation error is found to be constrained by the dissipation through activity switch in a universal way, which suggests that energetic allocation in different degrees of the system would affect the performance in a fundamental way.

Anti-icing Coating Inspired by Ice Skating

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Abstract: Accumulation of ice to surfaces brings dangerous and costly problems to our daily life. Thus there has been great interesting in finding an effective method to fight against icing. At the surface of frozen water, even at temperatures below 0 °C, ice's hexagonal structure breaks down and forms a liquid-like layer that lubricates the surface, allowing figure skaters to spin and glide. In this paper, we report an anti-icing coating inspired by ice skating. Hyaluronic acid is used in the anti-icing coating to form aqueous lubricating layer benefitting from its high water absorbing property. Dopamine, the main component of the mussel adhesive protein, is introduced to anchor the hyaluronic acid to the solid surfaces to render the coating applicable to all types of surfaces. At the same time it serves as the crosslinking agent for hyaluronic acid, thus the thickness of the water collecting film could be easily varied. Ice adhesion strength on surfaces coated with such kind of coating could be more than one order of magnitude lower than that of uncoated ones. The results indicate that this anti-icing coating with an aqueous lubricating layer has great potential for fighting against icing problems.

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水和水溶液微观结构的定量拉曼光谱研究

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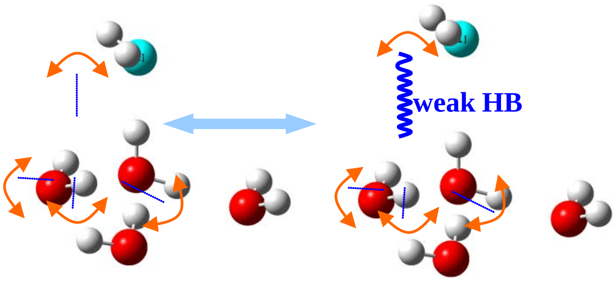
摘要：水和各种水溶液是人类赖以生存的物质，这些溶液的微观结构对认识其宏观性质很重要。这些水和水溶液微观结构的研究已经超过了 100 年，但是依旧不清楚它们的微观结构。这里我们提出了新的拉曼定量光谱分析技术，利用这种技术首次定量地给出水和各种水溶液的微观结构。例如我们提供了液体水中确实有冰状水的直接实验证据，并且我们发现这种冰状水的结构随着温度的升高也会有一些调整，除此之外水中还有部分水分子处于氢键松散的状态，这两部分水的晗，熵的差距随着温度的升高而升高。 再如我们获得了水溶液中溶质周围的水分子数目。对比不同溶质，不同浓度下第一溶剂层水分子数目，我们解释了卤素阴离子和碱金属阳离子形成离子对的情况，我们发现在 0.1 M/L 极稀情况下这些盐除了钠盐外都形成明显的直接接触离子对，且随着浓度越大，离子对越多。我们还分析了丙酮水溶液的微观结构，获得了丙酮周围水分子的光谱，给出了丙酮周围水的结构及其与浓度的关系，通过这些结构了解了有机物在水中的溶解机理。这些研究表明，我们提出的定量拉曼光谱分析技术是研究水和水溶液的微观结构的强有力工具。

关键词：水，盐水溶液，丙酮水溶液，拉曼光谱，定量分析



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自然沙堆积的静止角研究

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摘要：本文以塔克拉玛干沙漠西南边缘的自然沙丘的沙子为研究对象，对不同粒径的沙采用漏斗法进行沙堆积，并录像记录了沙的堆积过程。最后将录像处理成图片，用计算软件“CorelDraw”处理，从而得到沙堆静止角和崩塌角随时间和沙粒粒径的变化关系。得出结论：（1）沙堆的崩塌角和静止极角随时间的变化是振荡变化。首先，静止角逐步变大到崩塌角，崩塌后堆积角回到静止极角，然后再增大到崩塌角，如此往复。(2) 当粒径小于 0.30mm 时，沙堆崩塌角及崩塌角与静止极小角的差值随沙粒粒径的增大而增大；但当粒径大于 0.30mm 时，其差值随沙粒粒径的增大而减小。（3）崩塌角与静止极角的差值的平均值为（4.6±0.6）°（4）混合沙的堆积静止角与崩塌角的差值的变化范围为 33.5°～39.8°．

Research on the angle of repose of natural sand

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Abstract: In this paper we take the sands collected from the natural dunes at the southwest edge of Taklimakan desert as our experimental subjects. We drift the sands into mounds by using static funnel method and record some videos for the drifting processes. Then we translate the videos into pictures and analyze them by the computer software “CorelDraw”. By analysis we get the Dependence of the static angle and the collapse angle of the sand mounds on the time and the particle size. Then we make some conclusions: (1) The angle of the sand mound always follow the same circle, i.e., from the maximum static angle to the collapse angle and back to the maximum static angle. Thus both the collapse angle and the maximum static angle oscillate over time. (2) When the particle diameter is less than 0.30 millimeter, the difference between the collapse angle and the static angle will be increased with the increase of the particle size. Whereas when the particle diameter is greater than 0.30 millimeter, it will be decreased with the increase of the particle size. (3) The average difference between the collapse angle and the static angle is （4.6±0.6）°. (4) The difference between the collapse angle and the static angle of the mixed sand mounds is ranged from 33.5 °to 39.8°.

Keywords: particulate matter; static angle; collapse angle; sand; sand heap

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体积水中水分子转动跳跃与平动的关联

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摘要：我们用分子动力学模拟的方法研究了体积水中水分子转动跳跃(jump reorientations)与平动扩散的关联。我们发现，转动跳跃会使水分子及其邻近水分子处在短暂的快速平动之中，而在没有转动跳跃发生时，水分子平动较慢。这些转动跳跃还会在局域连续发生，使水分子在较短的时间内产生很大的平动位移。对不同时长的水分子运动轨迹的统计分析发现，这种由转动跳跃带来的快速运动对应的位移贡献了水分子平动总位移的大约 70%，占用的时间仅为总时间的约 40%。进一步，我们发现转动跳跃对局域不同位置的水分子的平动的影响程度不同：其中发生转动跳跃的水分子自身平动加强较大，与之相邻的氢键受体水分子次之，而与之相邻的氢键供体水分子平动加强较小。并且，相比于单次的转动跳跃，连续发生的转动跳跃能更大幅度地促进局域水分子的平动。依此我们提出一个水分子扩散运动的图像，其中平动伴随着转动同时发生。这些结果能使我们更好地理解水分子的微观运动模式，并有助于水分子扩散运动的机制的研究。

关键词：水分子，关联，转动跳跃，平动，分子动力学模拟

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