2021 Soft Matter and Biophysics Seminars, ITP-CAS

Monday 01 March 2021 - Tuesday 01 March 2022

Institute of Theoretical Physics, Chinese Academy of Sciences

Programme

磁驱动软体薄膜微型机器人的路径跟踪与多模态运动

报告人：徐天添 中国科学院深圳先进技术研究院 研究员
地点：ITP 6620

摘要：微型机器人，大到几毫米，小到几微米，可以很轻松地在复杂狭小的空间作业。生物相容性好且材料质地柔软的可实现多模态智能运动的微型机器人，在生物工程学和体内靶向治疗方向有非常大的应用潜力。现有的磁驱动微型机器人仍停留在简单驱动控制，如何实现精准的运动控制以解决实际问题是目前面临的巨大挑战。报告将围绕着软体薄膜微型机器人的运动控制和运动特性展开，介绍磁驱动软体薄膜微型机器人的视觉伺服三维路径跟踪控制，以及适应复杂环境的多模态运动机制。

Designing the Morphology of Separated Phases in Multicomponent Liquid Mixtures

报告人：毛晟 北京大学助理教授、特聘研究员
地点：ITP 6620

Abstract: Phase separation of multicomponent liquid mixtures plays an integral part in many processes ranging from industry to cell biology. While the physics of binary and ternary liquid mixtures is well-understood, the thermodynamic properties of N-component mixtures with N>3 remains relatively unexplored. This makes it challenging to understand how cells control concentrations of molecules and their interactions to navigate phase diagrams to achieve target structures. To address this issue, we developed novel algorithms for constructing phase diagrams and for predicting the morphology of separated phases. To determine the number of coexisting phases and their compositions, we developed a new algorithm for constructing complete phase diagrams, based on numerical convexification of the discretized free energy landscape. Furthermore, we developed a graph theory approach to predict the topology of coexisting phases from a given set of surface energies (forward problem), enumerate all topologically distinct morphologies, and reverse engineer conditions for surface energies that produce the target morphology (inverse problem).

弹性体—纳米颗粒复杂体系的理性设计与性能优化

报告人: 刘军 教授，北京化工大学
地点： ITP 6620

摘要：面向高性能弹性体材料的重大需求，报告人长期致力于弹性体-纳米颗粒复杂体系的热力学与动力学、结构演化与力学响应的计算模拟研究。针对力学性能与自修复，发展了计算模拟方法与提出了等效性原理。明确了 Stokes-Einstein**方程描述纳米颗粒在大分子链中扩散运动的规律，揭示了纳米粒子在大分子链中的分散相图，明晰了分子链与纳米粒子界面作用机制，提出了橡胶纳米力学增强的逾渗理论与调节橡胶粘弹性的新策略, 优化出橡胶纳米复合材料的“理想网络” 新结构。本报告将主要介绍我们最近的两个工作：利用分子动力学模拟研究纳米粒子在聚合物交联网络中的扩散动力学规律，以及全弹性体基(all-elastomer based)纳米复合材料的计算模拟设计与性能优化。**

Bioinspired Colloidal Motors for Biomedical Applications

报告人: 贺强 教授，哈尔滨工业大学
地点： ITP 6620

Abstract: Self-propelled colloidal motors have great potential in the biomedical field such as active target delivery, detoxification, minimally invasive diagnostics, and nanosurgery, owing to their tiny size, autonomous motion, and navigation capacities. To enter the clinic, biomedical colloidal motors request the biodegradability of their manufacturing materials, the biocompatibility of chemical fuels or externally-physical fields, the capability of overcoming various biological barriers. I will first introduce the recent advances of synthetic colloidal motors based on controlled chemical self-assembly and how such a strategy permits the realization of synthetic motors with the engineering features, such as sizes, shapes, composition, self-propulsion, collective motion and other functions. Next, I will talk how these chemically assembled motors could be designed to overcome the mentioned biological barriers. The challenges and future research priorities will be also addressed.

带电软物质

Speaker**报告人 陈光（北京大学先进制造与机器人系）**
Date**日期** 2021/06/29 15:00-17:00
Venue**地点 南楼6620会议室**
Abstract**摘要**
带电软物质在自然界和生产活动中是无处不在的。许多高分子、胶体、表面活性剂等软物质体系在水溶液中都会因电离现象而产生复杂的静电相互作用，同时也被赋予了特殊的功能。如细胞膜上的膜蛋白利用静电相互作用调节离子通道的选择透过性；柔性电子常用的水凝胶因静电相互作用而具有pH敏/盐敏刺激响应型的溶胀收缩行为和导电效果；聚电解质溶液的流变学特性也因复杂的静电相互作用而一度成为高分子物理与食品日化工业的难题。报告人将阐述带电软物质特殊功能的产生机制，介绍带电软物质的物理理论和功能材料在柔性电子中的应用。

邀请人：孟凡龙

用于细胞组织冻存的仿生控冰新材料

报告人 王健君研究员（中国科学院化学研究所）
日期 2021年08月31日 15:00
地点 北楼322会议室
摘要
冷冻保存是将细胞、组织及器官等生物样品置于超低温环境中，大大降低其新陈代谢速率以实现长期存储，并能在解冻后恢复生物样品功能的科学与技术。冷冻保存是目前细胞治疗、再生医学及器官移植等先进医疗技术能否充分发挥挽救生命潜力的瓶颈。目前广泛使用的玻璃化冷冻保存方法可以将生物样品内超过70%的水在冻存过程中变成玻璃态的水，避免冰晶的形成，从而保护生物样品免受冰冻伤害。但是该冷冻保存方法存在两大问题：1）玻璃化冻存必须添加大量具有细胞毒性的分子，如二甲基亚砜等，使生物样品在冻存后功能受损、复苏率不理想；2）组织或者器官的细胞成分多样、结构复杂，使用现有的冻存方法解冻复苏后无法有效恢复其生物功能。控冰蛋白能够控制冰晶成核与生长，可使自然界生活于酷寒地区的生物免受冰冻伤害。课题组受控冰蛋白启发开展了系列研究工作，明确了控冰蛋白尺寸对冰核形成的影响，揭示了控制冰晶生长的分子机制。并仿生创

制了系列控制冰晶形成的人体安全的材料，用于细胞组织的冻存，完全摒弃了二甲基亚砜等有毒分子的使用；研究显示仿生控冰材料冻存的细胞功能远优于玻璃化冻存的细胞。

报告人简介：

2006年10月在德国美因茨大学获得博士学位。

2007年5月起，在德国马普高分子所担任课题组长。2010年2月回中国科学院化学研究所工作，任研究员/课题组长。获基金委杰出青年基金项目、重点项目等支持。近年来主要开展冰晶形成分子机制研究、控冰新材料的创制并应用于防覆冰涂层与细胞、组织和器官的低温保存等领域。近五年发表论文包括Nature、Adv.Mater.、Angew.Chem.Int.Ed.、PNAS、J.Am.Chem.Soc.、Nat.Commun.、Sci. Adv.等。申请PCT专利9项，已获授权中国发明专利10余项。研究工作受到了国内外同行的广泛关注，得到了2014年美国物理学会三月年会的亮点报道，《高分子学报》编委；韩国高丽大学冰水研究中心顾问等。中国科学院分子科学中心第五届学术委员会委员；中国化学会第十三届理事会高分子学科委员会委员。

Percolation transition on multiplex networks

题目 Percolation transition on multiplex networks
报告人 李明（中国科技大学工程科学学院）
日期 2021/10/15 9:00-10:00
地点 北楼322会议室
摘要
The structure of interconnected systems and its impact on the system dynamics is a much-studied cross-disciplinary topic. Although various critical phenomena have been found in different models, study of the connections between different percolation transitions (continuous and discontinuous transitions) is still lacking. In this talk we will propose a unified framework to study the origins of the discontinuous transitions of the percolation process on interacting networks.

邀请人：孟凡龙

The role of hidden structural characteristics in glass-forming liquids: Two basic elements

主题：The role of hidden structural characteristics in glass-forming liquids: Two basic elements
报告人： 童华（中国科技大学物理学院）
日期： 2021年10月15日 15:00
地点： 北楼322会议室
摘要
Glass transition takes place when a liquid is cooled fast enough to avoid crystallization, during which the viscosity (or structure relaxation time) increases by many orders of magnitude over a narrow temperature window, but without obvious structural change. The possible role of structural ordering in the drastic dynamical slowing down has been intensively discussed over the decades but remains elusive, due to the intrinsic difficulty in the description of the complex liquid structure. Here we tackle this fundamental problem by showing that two basic elements are essential to identify the role of hidden structural characteristics in glass-forming, namely a proper structural order parameter and a nonlocal scenario for the structure-dynamics correlation.

First, we introduce a new structural order parameter characterizing local packing capability and show that the fast relaxation is controlled by the structure at local level while the slow relaxatiuon is controlled by structural ordering at static correlation length . This result crucially establishes that the two key relaxation modes at two characteristic time scales are the consequence of the presence of

the two intrinsic length scales in the structure.

Then, we show quantitatively that the growth of structural order when approaching the glass transition can be described by a linear scaling law as a function of temperatur, which leads to a universal Vogel-Fulcher-Tammann (VFT)-like relation between the relaxation time and the structural order parameter. More importantly, we find, based on the nonlocal scenario of structure-dynamics correlation, that such an intriguing VFT-like relation to be valid even at a particle level. We expect this nonlocal mechanism of structure relaxation, in addition to the hidden structural ordering, to be two essential ingredients for a complete theoretical description of the glass transition as a special type of thermodynamic phase transition.

邀请人：孟凡龙

蛋白质动力学与进化之间的对应关系

主题：蛋白质动力学与进化之间的对应关系 Dynamics-Evolution Correspondence in Protein Structures
报告人 唐乾元（日本理化学研究所（RIKEN）脑科学研究中心）
日期: 2021年11月25日 10:00
地点: Zoom meeting ID: 82181080836 Password: 125027
摘要
摘要：蛋白质的动力学和进化是生命科学研究中两个重要的研究主题。动力学和进化分别涉及到了生命现象中两个相差巨大的时间尺度，然而，许多研究表明，蛋白质短时间尺度的动力学和长时间尺度的遗传进化之间存在很高的相似性。为了揭示这种相似性的成因，我们提出了一个简化的理论模型框架，建立起了蛋白质动力学与进化之间的对应关系，并用真实的蛋白质结构数据进行了验证。在这个模型的基础上，我们还进一步分析了生物系统的“功能敏感性”和“突变稳定性”二者之间的关系。研究表明，尽管蛋白质的功能运动涉及到大量的自由度，但构成蛋白质的各个氨基酸却会形成某种集体秩序，倾向于沿着少数几个特定的方向协同运动，以便其发挥功能，而这几个特定的方向是进化稳定的，突变所影响的主要是其它非主导的方向。这种对应关系也对我们研究其它生命系统（例如大脑、生物网络）乃至更一般的复杂系统也具有重大的启发性。

Tang, Q. Y., & Kaneko, K. (2021). Dynamics-Evolution Correspondence in Protein Structures. Physical Review Letters, 127(9), 098103.

唐乾元，现为日本理化学研究所（RIKEN）脑科学研究中心研究员，南京大学物理学博士。主要研究方向为统计物理在蛋白质、大脑等生命科学问题中的应用，在 Phys. Rev. Lett.，Phys. Rev. Research，PloS. Comp. Biol. **等杂志发表过多篇论文。科普作者（笔名：傅渥成），知乎物理学、生物学领域优秀回答者，曾出版科普书《宇宙从何而来》。**

Studies of transport processes in atomic/molecular systems: progress report

Title**题目** Studies of transport processes in atomic/molecular systems: progress report
Speaker**报告人 崔冰宇 博士 （宾夕法尼亚大学化学系）**
Date**日期** 2021年11月29日 10:00-11:30
Venue**地点 腾讯会议：**913-110-123
Abstract**摘要**
This talk consists of three parts:

Phonon transport: elastic materials experience internal resistance to the deformation caused by external forces, which is characterized by a stress-strain curve. Most theories of elastic constants are established on the linear region of the stress-strain curve. The affine elastic constants were

studied in detail in the work of Born and Huang (BH). Later, its nonaffine corrections were developed by Lemaitre and Maloney (LM). Reviewing the BH theory, and comparing it with LM formalism, I will show that they address the elasticity problem from two complementary angles: LM approach works by identifying the local nonaffine forces while BH arguments are based on optimization of local nonaffine displacements. The linear regime of the stress-strain curve is also vital for elastic waves. In (elastic) disordered systems, depending on the scale of wavelength, the damping coefficient of sound waves might exhibit different behaviors. I will provide analytical results, supported by numerical evidence, of the dependence of the damping coefficient on the wavenumber, for sound waves propagating in systems having quenched disorder. The vibrational density of states of amorphous systems are also featured by these waves.

Electron-transfer-induced heat transport (ETIHT): electron transfer is a fundamental process that drives many physical, chemical, and biological transformations. The semiclassical Marcus theory is the most common approach used for understanding such phenomena. Based on the Marcus theory, it was recently found that electron transfer between molecular sites characterized by different local temperatures is associated with heat transfer between these sites and thus contributes to heat conduction in such systems. However, Marcus theory is based on a high temperature approximation that fails at low temperatures where nuclear tunneling becomes important. I will provide, within a simple model, a unified framework that includes the deep (nuclear) tunneling limit of electron transfer and the associated heat transfer, thereby, extending the ETIHT theory to the low temperature limit.

Photochemical processes in the strong light-matter coupling limit: light-matter interaction in confined geometries often shows characteristic signatures such as the Purcel effect on the decay rate of molecular excitations and Rabi splitting of optical transitions. Such phenomena are analyzed for systems comprising 2-level atoms by the Tavis-Cummings model. To describe behavior of molecules in such situations an extended model is needed that includes the effect of nuclear motion. I will describe our current work to investigate the interplay between the many-molecule optical response and the local (single molecule) nuclear dynamics with possible consequences to molecular photochemistry.