软物质数学建模和方法研讨会

会议介绍：

上海交通大学将于 2021 年 6 月 1 日举办软物质数学建模与方法研讨会。此次研讨会将邀请华东理工大学化工学院练成研究员、纽约大学库朗所干则成博士和上海交通大学物理与天文学院袁家兴博士，介绍微纳尺度界面问题的数学建模及其方法，以及软物质体系的多尺度方法。与会者将共同探讨相关数学模型和快速算法在电化学能源、生物大分子等科学问题中的应用。

会议组织：　上海交通大学数学科学学院快速算法和高性能计算实验室

会议地点：　上海交通大学（闵行校区）理科群楼 6 号楼 437 会议室

会议联系人：高伟航，gaowh2019@sjtu.edu.cn

报告安排（6 月 1 日，周二）

时间	报告主题	报告人	报告人单位
13:30-14:15	电化学过程的多尺度多物理场建模	练成	华东理工大学
14:20-15:05	Spectral EHD solver for computer simulations of charged spherical particles	干则成	纽约大学
15:05-15:25	交流讨论		
15:25-16:10	Dielectric effects and charge regulation in polyelectrolyte materials	袁家兴	上海交通大学
16:10—16:30	自由讨论		

报告题目和摘要

报告 (1)

题目：电化学过程的多尺度多物理场建模

演讲人：练成 （华东理工大学化工学院）

摘要：我国有着丰富的可再生能源，可再生能量的高效储存和应用可以助力碳中和，超级电容器/锂离子电池/燃料电池等是众多储能技术应用较为广泛，但他们的效应仍需提高，亟需发展电化学过程的多尺度多物理场建模方法和软件，理性设计电极/电解液。这里我们发展了多尺度多物理场动态密度泛函理论，明确外场作用下多孔电极中传质-反应耦合机制，实现电化学材料结构与电化学性能的定量关联，为新型电极材料和电解液的开发提供理论依据。

报告 (2)

题目：Spectral EHD solver for computer simulations of charged spherical particles

演讲人：干则成（纽约大学库郎所）

摘要：Varies complex systems in nature, such as colloids, membranes and biomolecules, can be modeled as particles under ElectroHydroDynamics (EHD) interactions. In this talk, we will introduce coarse-grained models for simulating such systems, and then describe fast spectral methods combining analytical reduction and efficient numerical techniques based on the Fast Multipole Method (FMM) and FFTs, that can compute electrostatic and hydrodynamic interactions in linear time in the number of particles.

报告 (3)

题目：Dielectric effects and charge regulation in polyelectrolyte materials

演讲人： 袁家兴（上海交通大学物理与天文学院）

Abstract: Understanding the long-ranged and many-body electrostatic interactions has always been a frontier topic in the field of soft matter, ranging from polyelectrolytes and biomolecules to charged nanoparticles and membranes. Dielectric effects and charge regulation are widely encountered in charged soft matter, the former of which arises when the fluid solvent and the macromolecular surface has a permittivity contrast while in the latter case the net charge of solvated entities is not constant but instead depends on the local dissociation equilibrium of individual ionizable groups. Despite their important role, dielectric effects and charge regulation are rarely taken into account in theoretical and computational studies due to the lack of appropriate and efficient solvers. In this talk, I will review the recent development of computational methods that handle these two effects, followed by their applications in investigating the equilibrium and dynamic properties of polyelectrolyte materials, including polyelectrolyte brushes (grafted polyelectrolytes) and polyelectrolyte hydrogel.