



## 会议告知

化学工程国家联合重点实验室-华理分室和华东理工化工学院联手于 2016 年 9 月 23-25 日共同主办介尺度问题研究进展国际研讨会 (英文名称 “International Workshop on Advances in the Studies of Mesoscale Problems”). 会议瞄准国内外关于介尺度问题研究的前沿和最新进展, 旨在为该领域研究人员提供一个思想碰撞和学术交流的平台。会议内容丰富, 欢迎各位老师和研究生参加。

### ❖ Agenda (日程安排)

**Venue: 16th Research Building, Room 110 (实验十六楼 110)**

	Time	Topic	Speaker	Chair
Morning, Sept. 24	08:30-08:40	Introduction and Welcome	Honglai Liu	Umberto Marini Bettolo Marconi
	08:40-9:30	Confinement-induced high pressure phases in nanopores. Can the pressure be in the Megabar range?	Keith E. Gubbins	
	9:30-10:10	Stability-constrained multi-scale models for complex flows	Wei Ge	
	10:10-10:30	Coffee Break		
	10:30-11:20	Towards a statistical mechanical theory of active fluids	Umberto Marini Bettolo Marconi	Nick Quirke
	11:20-12:00	Development and Application of Static and Dynamic Classical Density Functional Theory for Capacitive Energy Storage	Cheng Lian	
	12:00	Lunch		
Afternoon, Sept. 24	13:30-14:20	Study of Hydrated Ions Transport in Ion-exchange membranes: role of morphology	Liang Wu	Shuangliang Zhao
	14:20-15:00	Surface Wettability Effect on Fluid Transport in Nanoscale Slit Pores	Yaofeng Hu	
	15:00-15:20	Coffee Break		

	15:20-16:00	Modeling Studies of Biogas Purification and Bio-CH <sub>4</sub> Storage	Linghong Lu	Wei Ge
	16:00-16:40	Molecular modeling of biomolecules translocation through nanopores	Jiawei Shen	
	16:40-17:20	Mesoscale concept for turbulence modeling and simulation	Lin Zhang	
		Banquet		

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	Time	Topic	Speaker	Chair
Morning, Sept. 25	8:30-9:20	Excess electron states in fluid methane: Density-functional versus Lanczos approaches	Nick Quirke	Shuangliang Zhao
	9:20-10:00	Computational Simulation of Supported Nanocatalysts under Realistic Conditions	Jianguo Wang	
	10:00-10:30	Coffee Break		
	10:30-11:10	Meso-scale Structures in Ionic Liquids Systems: Ionic Cluster and Hydrogen Bond	Xiaomin Liu	Jianguo Wang
	11:10-11:50	Study of reaction and transport at surfaces of graphene	Yingchun Liu	
	12:00-13:30	Lunch		
Afternoon, Sept. 25	13:30-14:10	Assembly of polyelectrolytes: towards soft nanoparticles for functional materials	Junyou Wang	Marc Pera-Titus
	14:10-14:50	A theoretical understanding of amino acid interaction with graphene and its derivatives	Liangliang Huang	
	14:50-15:20	Coffee Break		

	15:20-16:00	Dynamics of Pickering emulsions in the presence of an interfacial reaction: a simulation study	Marc Pera-Titus	Liangliang Huang
	16:00-16:40	Ordered Water Monolayer That Does Not Completely Wet Water and Molecular-scale Hydrophilicity at Room Temperature	Chunlei Wang	
	16:40-17:20	The Role of Polymer-Substrate Interaction Strength in Polymer Films on Solid Substrates: the Glass Transition and Friction Force	Rong An	
		Banquet		