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澳大利亚研究理事会激子科学卓越中心 (ARC Centre of Excellence in Exciton Science), 化学系, 悉尼大学

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### 教育和工作经历

- **2017.09 – 至今** 澳大利亚悉尼大学 化学系 博士后研究员  
澳大利亚研究理事会激子科学卓越中心  
导师: Dr. Asaph Widmer-Cooper
- **2014.11 – 2016.11** 英国剑桥大学 化学系 联合培养博士研究生  
导师: Prof. Daan Frenkel [时任剑桥大学化学系主任。荷兰皇家科学院院士 (1998), 美国艺术与科学学院院士 (2008), 第三世界科学院院士 (2012), 英国皇家科学院外籍院士 (2006) 以及美国国家科学院外籍院士 (2016)。2016 年获得国际纯粹及应用物理联合会 (IUPAP) 玻尔兹曼奖章 (剑桥历史上第二位)。]
- **2010.09 – 2017.07** 北京化工大学 化学工程学院 硕士/博士研究生  
北京软物质科学与工程高精尖创新中心  
有机无机复合材料国家重点实验室  
导师: 张现仁教授
- **2006.09 – 2010.07** 北京化工大学 化学工程学院 本科生

### 研究方向

- 研究固-液界面/液-液界面处由浓度或温度梯度引起的流体运动 (如 Marangoni 效应、扩散泳、热泳), 理解界面附近质量传递、热量传递与动量传递的耦合与依赖性。
- 与墨尔本大学、莫纳什大学及悉尼大学多个实验课题组合作研究用于太阳能吸收与转化等应用领域的分子/纳米材料 (如  $\pi$ -共轭分子、金纳米球、金纳米棒等) 自组装过程, 利用多尺度模型和模拟的手段研究实验体系中的热力学稳定态, 流体及颗粒运动, 和反应机理等问题。
- 与天津大学实验课题组合作研究用于水处理、燃料电池等应用领域的新型高性能分离膜 (如氧化石墨烯膜、COF 膜) 的研究与开发, 利用分子模拟和介观模拟研究膜材料中纳米限制空间内的流体运动与分离, 优化膜材料的渗透性和选择性。
- 研究固-液界面上表面纳米气泡/液滴的热力学性质和动力学演化过程, 通

过调控表面纳米气泡形态控制固-液界面处流体的性质与行为。

研究成果在 **Phys. Rev. Lett.**、**Adv. Funct. Mater.**、**J. Chem. Phys.**等杂志发表论文共 34 篇，其中一作和通讯论文共 16 篇。

## 主要研究成果及发表论文

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[Marangoni 效应、扩散泳、热泳的相关研究，从微观尺度上预测界面附近由浓度梯度或温度梯度引起的流体运动速度。]

1. **Microscopic Marangoni flows cannot be predicted on the basis of pressure gradients.** Y Liu, R Ganti, HGA Burton, X Zhang, W Wang, D Frenkel – **Phys. Rev. Lett.** 119, 224502 (2017) [北京化工大学首篇以本校学生为第一作者，北京化工大学为第一署名单位在此期刊发表的论文，被学校新闻网站报道。]
2. **Hamiltonian Transformation to Compute Thermo-osmotic Forces.** R Ganti, Y Liu, D Frenkel – **Phys. Rev. Lett.** 121, 068002 (2018)
3. **Molecular simulation of thermo-osmotic slip.** R Ganti, Y Liu, D. Frenkel – **Phys. Rev. Lett.** 119, 038002 (2017)
4. **Pressure gradients fail to predict diffusio-osmosis.** Y Liu, R Ganti, D Frenkel – **J. Phys. Condens. Matter** 30, 205002 (2018)

[分子/纳米材料自组装的相关研究，通过静电作用和表面结构修饰实现纳米颗粒的定向定位自组装，通过各种手性光测量手段理解手性纤维分子的自组装机理。]

5. **Direct Assembly of Vertically Oriented, Gold Nanorod Arrays.** H Zhang, Y Liu, M F S Shahidan, C Kinnear, F Maasoumi, J Cadusch, E M Akinoglu, T D James, A Widmer-Cooper, A Roberts, P Mulvaney – **Adv. Funct. Mater.** 31, 2006753 (2020) [IF: 16.836]
6. **The Role of Fiber Agglomeration in Formation of Perylene-Based Fiber Networks.** A Sharma, J P Wojciechowski, Y Liu, T Pelras, C M Wallace, M Müllner, A Widmer-Cooper, P Thordarson, G Lakhwani – **Cell Rep. Phys. Sci.** 1, 100148 (2020)
7. **Self-Assembly of Spherical and Rod-Shaped Nanoparticles with full Positional Control.** J A Lloyd, Y Liu, S H Ng, T Thai, D E Gómez, A Widmer-Cooper, U. Bach – **Nanoscale** 11, 22841 (2019)

[新型高性能分离膜的相关研究，通过构建膜材料孔内的化学及物理非均匀性，借助表面纳米气泡实现超快高选择性水渗透膜。]

**Manipulating chemical and geometrical heterogeneities of graphene oxide surface**

**for fast selective water flow.** Y Ma, R Zhang, Y Liu, Y Yang, B Shi, X You, J Shen, D Yin, H Wu, Z Jiang – Nat. Commun. *Under review*

[表面纳米气泡/液滴的相关研究，提出的接触线锚定机理在该领域内被广泛接受和研究。相关论文引用量超过 200 余次，多张图被 Reviews of Modern Physics(IF: 45.037)综述文章(Rev. Mod. Phys. 87, 981, 2015)采用。]

**8. Nanobubble stability induced by contact line pinning.** Y Liu, X Zhang – **J. Chem. Phys.** 138, 014706 (2013)

**9. Evaporation dynamics of nanodroplets and their anomalous stability on rough substrates.** Y Liu, X Zhang – **Phys. Rev. E** 88, 012404 (2013)

**10. A unified mechanism for the stability of surface nanobubbles: Contact line pinning and supersaturation.** Y Liu, X Zhang – **J. Chem. Phys.** 141, 134702 (2014)

**11. Contact line pinning and the relationship between nanobubbles and substrates.** Y Liu, J Wang, X Zhang, W Wang – **J. Chem. Phys.** 140, 54705 (2014)

**12. Molecular dynamics simulation of nanobubble nucleation on rough surfaces.** Y Liu, X Zhang – **J. Chem. Phys.** 146, 164704 (2017)

**13. Stability of Pinned Surface Nanobubbles Against Expansion: Insights from Theory and Simulation.** Y Liu, S Bernardi, A Widmer-Cooper – **J. Chem. Phys.** 153, 024704 (2020)

## 其他研究成果及发表论文

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[一作或通讯论文，针对研究体系开发的模型或计算方法，以及在研究过程中遇到的相关问题的探索，如线张力效应、气液相变成核等。]

**14. A dissipative particle dynamics model for studying dynamic phenomena in colloidal rod suspensions.** Y Liu, A Widmer-Cooper – **J. Chem. Phys.** Accepted (2021)

**15. Coarse-grained simulation of the translational and rotational diffusion of globular proteins by dissipative particle dynamics.** J Wei<sup>[通讯]</sup>, Y Liu<sup>[通讯]</sup>, F song – **J. Chem. Phys.** 153, 234902 (2020)

**16. A Versatile Simulation Method for Studying Phase Behavior and Dynamics in Colloidal Rod and Rod-Polymer Suspensions.** Y Liu, A Widmer-Cooper – **J. Chem. Phys.** 150, 244508 (2019)

**17. A review of recent theoretical and computational studies on pinned surface nanobubbles.** Y Liu, X Zhang – **Chin. Phys. B** 27, 14401 (2017)

**18. Vapor bridges between solid substrates in the presence of the contact line**

pinning effect: Stability and capillary force. [Y Liu](#), X Zhang – [J. Chem. Phys.](#) 145, 214701 (2016)

19. Accurate determination of the vapor-liquid-solid contact line tension and the viability of Young equation. [Y Liu](#), J Wang, X Zhang – [Sci. Rep.](#) 3, 2008 (2013)

20. Nucleation mechanism for vapor-to-liquid transition from substrates with nanoscale pores opened at one end. [Y Liu](#), Y Men, X Zhang – [J. Chem. Phys.](#) 137, 104701 (2012)

21. How nanoscale seed particles affect vapor-liquid nucleation. [Y Liu](#), Y Men, X Zhang – [J. Chem. Phys.](#) 135, 184701 (2011)

[非一作论文，指导组内学生的研究工作，包括表面纳米气泡、相变成核等。]

22. Surface Nanobubbles Nucleate Liquid Boiling. J Zou, H Zhang, Z Guo, [Y Liu](#), J Wei, Y Huang, X Zhang – [Langmuir](#) 34, 14096–14101 (2018)

23. Contact Line Pinning Effects Influence Determination of the Line Tension of Droplets Adsorbed on Substrates. H Zhang, S Chen, Z Guo, [Y Liu](#), F Bresme, X Zhang – [J. Phys. Chem. C](#) 122, 17184 (2018)

24. What experiments on pinned nanobubbles can tell about the critical nucleus for bubble nucleation. Q Xiao, [Y Liu](#), Z Guo, Z Liu, D Frenkel, J Dobnikar, X Zhang – [Eur. Phys. J. E](#) 40, 114 (2017)

25. How nanobubbles lose stability: Effects of surfactants. Q Xiao, [Y Liu](#), Z Guo, Z Liu, X Zhang – [Appl. Phys. Lett.](#) 111, 131601 (2017)

26. Solvent exchange leading to nanobubble nucleation: A molecular dynamics study. Q Xiao, [Y Liu](#), Z Guo, Z Liu, D Lohse, X Zhang – [Langmuir](#) 33, 8090 (2017)

27. Modeling the interaction between AFM tips and pinned surface nanobubbles. Z Guo, [Y Liu](#), Q Xiao, H Schönherr, X. Zhang – [Langmuir](#) 32, 751 (2016)

28. Hidden nanobubbles in undersaturated liquids. Z Guo, [Y Liu](#), Q Xiao, X. Zhang – [Langmuir](#) 32, 11328 (2016)

29. Vapour-to-liquid nucleation in cone pores. J Li, [Y Liu](#), G. Jiang, X. Zhang – [Molecular Simulation](#) 42, 1 (2016)

30. Constrained lattice density functional theory and its applications on vapor-liquid nucleations. Z Guo, [Y Liu](#), X. Zhang – [Sci. Bull.](#) 60, 320 (2015)

31. Stability of micro-Cassie states on rough substrates. Z Guo, [Y Liu](#), D Lohse, X Zhang, X Zhang – [J. Chem. Phys.](#) 142, 244704 (2015)

32. Mechanism of two-step vapour-crystal nucleation in a pore. J van Meel, [Y Liu](#), D

Frenkel – [Mol. Phys.](#) 113, 2742 (2015)

**33. Condensation of droplets on nanopillared hydrophobic substrates.** Q Guo, [Y Liu](#), G Jiang, X Zhang – [Soft Matter](#) 10, 1182 (2014)

**34. Cooperative effect in nucleation: Nanosized seed particles jointly nucleate vapor-liquid transitions.** Q Guo, [Y Liu](#), G Jiang, X. Zhang – [J. Chem. Phys.](#) 138, 214701 (2013)

## 交流访问

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**1. Molecular Simulation and Its Application in Nanoscale System.** – 姜忠义教授课题组, 天津大学, 在线会议, Jun. 4, 2020

**2. Modelling Electrophoresis of Rod-shaped Colloidal Particles.** – Prof. P. Mulvaney's group, University of Melbourne, 澳大利亚, Oct. 4-7, 2019

**3. Stability of Surface Nanobubbles.** – Prof. D. Lohse's group, University of Twente, 荷兰, Jan. 25-26, 2015

## 参加学术会议

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**1. Orientation of Gold Nanorods in Electrophoresis.** [口头报告](#) – 10<sup>th</sup> Australian Colloid and Interface Symposium, Sydney, 澳大利亚, Feb. 8-11, 2021

**2. Chiral Twist in Monolayer Assemblies of Rod-like Colloids.** [口头报告](#) – Statistical Mechanics of Soft Matter (SM<sup>2</sup>) 2020, Online, 澳大利亚, Dec. 14-16, 2020

**3. Dynamic Simulations of Rod-Shaped Colloidal Particles: Phase behaviour, self-assembly, diffusion and electrophoresis.** [口头报告](#) – ICONN2020, Brisbane, 澳大利亚, Feb. 9-13, 2020

**4. Dynamic Simulations of Rod-Shaped Colloidal Particles: Phase behaviour, self-assembly, diffusion and electrophoresis.** [口头报告](#) – ACEx Annual Workshop 2019, RMIT University, Melbourne, 澳大利亚, Dec. 9-11, 2019

**5. Dynamic Simulations of Rod-Shaped Colloidal Particles: Phase behaviour, self-assembly, diffusion and electrophoresis.** [口头报告](#) – Statistical Mechanics of Soft Matter (SM<sup>2</sup>) 2019, Adelaide, 澳大利亚, Dec. 16-17, 2019

**6. Dynamics Simulations of Rod-Shaped Colloidal Particles: Phase behavior, nucleation, and diffusion.** [口头报告](#) – ACEx Winter Workshop 2019, RMIT University, Melbourne, 澳大利亚, Jun. 28-29, 2019

**7. Stability and formation of surface nanobubbles: a computer simulation study.** [墙报](#) – 9<sup>th</sup> Australian Colloid and Interface Symposium, Hobart, Tasmania, 澳大利亚, Feb. 3-7, 2019

- 8. Modelling hard-rod suspensions for use in molecular-dynamics simulations.** 口头报告 – 9th Australian Colloid and Interface Symposium, Hobart, Tasmania, 澳大利亚, Feb. 3-7, **2019**
- 9. Molecular Dynamic Simulations of Hard Rod-Shaped Particles.** 口头报告 – Statistical Mechanics of Soft Matter (SM<sup>2</sup>) 2018, Auckland, 新西兰, Dec. 6-7, **2018**
- 10. Modelling hard-rod suspensions for use in molecular-dynamics simulations.** 口头报告 – Australian Symposium on Computational Enhanced Materials Design (ACEMD) 2018, Sydney, 澳大利亚, Jul. 22-25, **2018**
- 11. Pressure-gradient approach fails to predict the microscopic Marangoni flow and diffusio-osmosis.** 墙报 – Statistical Mechanics of Soft Matter (SM<sup>2</sup>) 2017, Sydney, 澳大利亚, Nov. 27-28, **2017**
- 12. Nanobubble stability induced by contact line pinning.** 口头报告 – Chinese Physical Society (CPS) Fall Meeting 2013, Xiamen, 中国, Sep. 13-16, **2013**
- 13. Nanobubble stability induced by contact line pinning.** 口头报告 – 2<sup>nd</sup> Chinese Meeting on Statistical Physics and Complex Systems, Qufu, 中国, Jul. 28-31, **(2013)**
- 14. Heterogeneous vapor-liquid nucleation and Nanobubble/droplet.** 墙报 – Chinese Physical Society (CPS) Fall Meeting 2012, Guangzhou, 中国, Sep. 20-23, **(2012)**

## 荣誉和奖励

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- 2017 北京化工大学优秀博士学位论文
- 2014 北京化工大学中外联合培养项目基金（赴剑桥大学）
- 2014 北京化工大学博士学位论文创新基金
- 2014 北京化工大学-“金发科技”奖学金
- 2013 （博士）研究生国家奖学金
- 2012 北京化工大学-金发科技社会资助（专项）奖学金
- 2012 （硕士）研究生国家奖学金