Yi-Xin Liu

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EDUCATION

PhD in Polymer Chemistry and Physics 2004 - 2009
Peking University (Top 2 in China), Beijing, China
Thesis: Phase Selection Pathways and Morphological Evolution in Polymer Crystallization: An Experimental and Theoretical Study on Low Molecular Weight Poly(ethylene oxide) Fractions
Advisor: Prof. Er-Qiang Chen

BS in Chemistry 2000 - 2004
Nanjing University (Top 5 in China), Nanjing, China

RESEARCH EXPERIENCE

Lecturer 2012 - present
Fudan University (Top 5 in China), Department of Macromolecular Science

- Directed self-assembly of block copolymers under soft confinements: nanostructures design and the mechanism of defect removal.
- Developing highly efficient numerical algorithms for computing self-assembly of block copolymers in bulk and under soft confinements.

Visiting Researcher (Advisor: Glenn H. Fredrickson) 2014 - 2016
University of California, Santa Barbara, Materials Research Laboratory

- Conducted complex Langevin field-theoretic simulations of polymeric materials under thermal fluctuations.
- Developed a density functional model for polymeric systems under thermal fluctuations.

Postdoctoral Fellow (Advisor: Hong-Dong Zhang) 2009 - 2012
Fudan University, Department of Macromolecular Science

- Developed high performance numerical methods for studying the equilibrium phase separation structures of charged block copolymers.
- Performed Monte Carlo simulations on the nucleation and growth process in thickening of monolayer poly(ethylene oxide) crystals in ultrathin films.

Graduate Student (Advisor: Er-Qiang Chen) 2004 - 2009
Peking University, College of Chemistry and Molecular Engineering

- Conducted phase field simulations on morphological evolution of monolayer poly(ethylene oxide) crystals.
- Carried out experimental studies on the nucleation, growth, thickening, and melting of monolayer poly(ethylene oxide) crystals in ultrathin films using in-situ atomic force microscopy.

RESEARCH INTERESTS

- Multiscale computer simulations and theoretical studies of complex fluids, e.g. block copolymers, polymer brushes, polyelectrolytes, and biological macromolecules in bulk and under confinements, and directed self-assembly of block copolymers (DSA).
- Numerical algorithms for field-theoretic simulations, molecular dynamics simulations, Monte-Carlo simulations, and phase field simulations.
- Ultrathin film polymer crystallization.

RESEARCH GRANTS

- **The General Program of the National Natural Science Foundation of China (NSFC):** Exploration and Design of Nontrivial Mesostructures of Polymeric Materials under Complex Conditions. PI, Expected, 800K RMB (120K USD) 2019-2022
- **Shanghai Pujiang Program:** Exploring Novel Nanostructures Through Mircophase Separation of Block Copolymers under Soft Confinements. PI, 200K RMB (30K USD) 2018-2020
- **The Young Scientists Fund of the National Natural Science Foundation of China (NSFC):** Computer Simulation Study of Pattern Formation in Ultrathin Film Polymer Crystallization. PI, 180K RMB (28K USD) 2011-2013
- **The Shanghai Postdoctoral Scientific Program:** Computer Simulation Study of Ordered Structures Self-Assembled from Concentrated Solutions of Weakly Charged Block Copolymers. PI, 40K RMB (6K USD) 2011-2011

PUBLICATIONS

Full text available: http://www.ngpy.org/publications

1. Song, J. Q.; **Liu, Y. X.***; Zhang, H. D. “Removal Pathways of Out-of-plane Defects in Thin Films of Lamellar Forming Block Copolymers.” **Macromolecules 2018**, *51*, 4201-4212.
2. Song, J. Q.; **Liu, Y. X.***; Zhang, H. D. “Theoretical Studies on Defect Removal in Block Copolymer Thin Film under Soft Confinement.” **Acta Polym. Sin. 2018**, DOI: 10.11777/j.issn1000-3304.2048.18907. (In Chinese)
3. **Liu, Y. X.***; Chen, E. Q. “Thickening Kinetics of Monolayer Crystals of Low Molecular Weight Poly(ethylene oxide) Fractions on Mica Surfaces.” **Acta Polym. Sin. 2018**, DOI: 10.11777/j.issn1000-3304.2017.17333. (In Chinese)

4. **Liu, Y. X.***; Zhang, H. D. “Structures and Surface States of Polymer Brushes in Good Solvents: Effects of Surface Interactions.” **Chinese J. Polym. Sci. 2018**, 36, 1047-1054.
5. Song, J. Q.; **Liu, Y. X.***; Zhang, H. D. “An Efficient Algorithm for Self-Consistent Field Theory Calculations of Complex Self-Assembled Structures of Block Copolymer Melts.” **Chinese J. Polym. Sci. 2018**, *36*, 488-496.
6. **Liu, Y. X.**; Delaney, K. T.; Fredrickson, G. H.* “Field-Theoretic Simulations of Fluctuation-Stabilized Aperiodic Bricks-and-Mortar Mesophase in Miktoarm Star Block Copolymer/Homopolymer Blends.” **Macromolecules 2017**, *50*, 6263-6272.
7. Song, J. Q.; **Liu, Y. X.***; Zhang, H. D. “A Surface Interaction Model for Self-assembly of Block Copolymers under Soft Confinement.” **J. Chem. Phys. 2016**, *145*, 214902.
8. **Liu, Y. X.***; Zhang, H. D. “On the Teaching of Modern Polymer Physics: I. Ginzburg Criterion.” **Polymer Bulletin 2015**, *1*, 73-79. (In chinese)
9. **Liu, Y. X.***; Zhang, H. D. “Exponential time differencing methods with Chebyshev collocation for polymers confined by interacting surfaces.” **J. Chem. Phys. 2014**, *140*, 224101.
10. **Liu, Y. X.***; Zhang, H. D.*; Tong, C. H.; Yang, Y. L. “Microphase Separation and Phase Diagram of Concentrated Diblock Copolyelectrolyte Solutions Studied by Self-Consistent Field Theory Calculations in Two-Dimensional Space.” **Macromolecules 2011**, *44*, 8261-8269.
11. **Liu, Y. X.**; Zhong, L. W.; Su, S. Z.; Chen, E. Q.* “Phase Selection Pathways in Ultrathin Film Crystallization of a Low Molecular Weight Poly(ethylene oxide) Fraction on Mica Surfaces.” **Macromolecules 2011**, *44*, 8819-8828.
12. Xie, H. L.; Wang, S. J.; Zhong, G. Q.; **Liu, Y. X.**; Zhang, H. L.*; Chen, E. Q.* “Combined Main-Chain/Side-Chain Liquid Crystalline Polymer with Main-Chain On the basis of Jacketing Effect and Side-Chain Containing Azobenzene Groups.” **Macromolecules 2011**, *44*, 7600-7609.
13. **Liu, Y. X.**; Chen, E. Q.* “Polymer crystallization of ultrathin films on solid substrates.” **Coord. Chem. Rev. 2010**, *254*, 1011-1037.
14. Xie, H. L.; **Liu, Y. X.**; Zhong, G. Q.; Zhang, H. L.*; Chen, E. Q.*; Zhou, Q. F. “Design, Synthesis, and Multiple Hierarchical Ordering of a Novel Side-Chain Liquid Crystalline-Rod Diblock Copolymer.” **Macromolecules 2009**, *42*, 8774-8780.
15. **Liu, Y. X.**; Li, J. F.; Zhu, D. S.; Chen, E. Q.*; Zhang, H. D.* “Direct Observation and Modeling of Transient Nucleation in Isothermal Thickening of Polymer Lamellar Crystal Monolayers.” **Macromolecules 2009**, *42*, 2886-2890.
16. Zhu, X. Q.; Liu, J. H.; **Liu, Y. X.**; Chen, E. Q.* “Molecular packing and phase transitions of side-chain liquid crystalline polymethacrylates based on p-methoxyazobenzene.” **Polymer 2008**, *49*, 3103-3110.
17. Zhu, D. S.; Shou, X. X.; **Liu, Y. X.**; Chen, E. Q.*; Cheng, S. Z. D. “AFM-tip-induced crystallization of poly(ethylene oxide) melt droplets.” **Front. Chem. China 2007**, *2*, 174-177.

18. Zhu, D. S.; **Liu, Y. X.**; Chen, E. Q.*; Li, M.; Chen, C.; Sun, Y. H.; Shi, A. C.*; Van Horn, R. M.; Cheng, S. Z. D.* "Crystal Growth Mechanism Changes in Pseudo-Dewetted Poly(ethylene oxide) Thin Layers." **Macromolecules 2007**, *40*, 1570-1578.
19. Zhu, D. S.; **Liu, Y. X.**; Shi, A. C.; Chen, E. Q.* "Morphology evolution in superheated crystal monolayer of low molecular weight poly(ethylene oxide) on mica surface." **Polymer 2006**, *47*, 5239-5242.
20. Zhu, D. S.; **Liu, Y. X.**; Chen, E. Q.*; Li, M.; Cheng, S. Z. D. "Pseudo-dewetting behavior of low molecular weight poly(ethylene oxide) melts on mica surface." **Acta Polym. Sin. 2006**, *9*, 1125-1128. (In chinese)
21. Zhu, D. S.; Shou, X. X.; **Liu, Y. X.**; Chen, E. Q.*; Cheng, S. Z. D. "AFM-tip-induced crystallization of poly(ethylene oxide) melt droplets." **Acta Polym. Sin. 2006**, *4*, 553-556. (In chinese)

PRESENTATIONS AND POSTERS

1. **Liu, Y. X.**; Delaney, K. T.; Fredrickson, G. H. "Density Functional Model for Fluctuating Polymer Solutions: Partial Saddle Point Approximation Approach." *Complex Fluid Design Consortium (CFDC) Annual Meeting*, Santa Barbara, California, **2016**
2. **Liu, Y. X.**; Delaney, K. T.; Fredrickson, G. H. "Density Functional Model for Fluctuating Polymer Solutions." *Complex Fluid Design Consortium (CFDC) Annual Meeting*, Santa Barbara, California, **2015**
3. **Liu, Y. X.** "Polymer Self-Consistent Field Theory in Bulk and under Confinement." *Invited Talk at ASML*, San Jose, California, **2014**
4. **Liu, Y. X.**; Zhang, H. D. "Exponential Time Differencing Methods for Numerical Self-Consistent Field Theory." *APS March Meeting*, Denver, Colorado, **2014**
5. **Liu, Y. X.** "Logarithmic-Normal Size Distribution in Crystallization of Polymeric Ultrathin Films Preceded by A Metastable Phase." *The 10th International Symposium on Polymer Physics*, Chengdu, **2012**
6. **Liu, Y. X.**; Zhang, H. D. "A Unified Computing Framework for Self-Consistent Field Theory: Applications in Charged Polymers." *Theory and Simulation on the Structure and Property of Macromolecular Systems Symposium*, Nanjing, **2012**
7. **Liu, Y. X.**; Zhu, D. S.; Chen, E. Q. "Phase Selection In Crystal Monolayer Of Low Molecular Weight Poly(Ethylene Oxide) On Mica Surface." *International Polymer Physics Workshop*, Xiamen, **2008**
8. **Liu, Y. X.**; Chen, E. Q. "Isothermal Thickening of PEO Lamellar Crystals on Mica Surface." *Polymer Symposium of China*, Chengdu, **2007**

HONORS AND AWARDS

- Scholarship awarded by China Scholarship Council 2014-2015
- Dongkong Scholarship for Graduates, Peking University 2008
- Student Award of Merit, Peking University 2008
- Renming Scholarship, Nanjing University 2000-2003

PROFESSIONAL MEMBERSHIPS AND ACTIVITIES

- Member: American Physical Society
- Reviewer: Polymer, Review of Scientific Instruments, Chinese Physics B

COMPUTATIONAL EXPERIENCE

- `Python`, `C/C++`, Parallel Programming (`MPI`, `GPU/CUDA`), `Matlab`, `HTML/CSS`, LaTeX.
- Familiar with `Linux`, `tensorflow`, `numpy/scipy`, `fftw`, `armadillo`, `blitz++`, `matplotlib`.
- Open source projects: polyorder - gyroid - ngpy - chebpy - mpltex

SUPERVISING AND MENTORING EXPERIENCE

Advisor
Department of Macromolecular Science, Fudan University

- Graduate student: Jun-Qing Song (PhD, 2018, not officially listed as the advisor due to university regulations).
- Undergraduate student: Zhi-Wei Xie (BS 2017).

TEACHING EXPERIENCE

Instructor: Polymer Physics 2014, 2017, 2018
Department of Macromolecular Science, Fudan University
Core undergraduate course, 30+ students, 15-week, 3-credit. Co-instructors: Hong-Dong Zhang and Jian-Feng Li.

Instructor: Introduction to Polymeric Materials 2016, 2017
Department of Macromolecular Science, Fudan University
Undergraduate course, 20+ students, 15-week, 2-credit. Co-instructor: Jia Guo.

Instructor: Quantitative Chemical Analysis Experiments 2006, 2007
College of Chemistry and Molecular Engineering, Peking University
Undergraduate experimental course, 17 students, 15-week, 2-credit.

References

Prof. Glenn H. Fredrickson — Postdoctoral Advisor (2014-2016)
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University of California, Santa Barbara
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Prof. An-Chang Shi — Collaborator
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