Curriculum Vitae

Yi-Xin Liu

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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 Experience

Lecturer, 2012 - present
Fudan University, 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 self-assembly of block copolymers in bulk and under soft confinements.

Visiting Researcher, 2014 - 2016
University of California, Santa Barbara, Materials Research Laboratory

- Field-theoretic simulations of polymeric materials under **thermal fluctuations**.
- Developing a density functional model for polymeric systems with fluctuations in consideration.

Postdoctoral Research Fellow, 2009 - 2012
Fudan University, Department of Macromolecular Science

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

Ph.D. Candidate, 2004 - 2009
Peking University, College of Chemistry and Molecular Engineering

- Phase field simulations on morphological evolution of monolayer PEO crystals.
- Experimental studies on the nucleation, growth, and thickening of monolayer PEO crystals in ultrathin films using in-situ atomic force microsocpy.

Education

Peking University, Beijing, 2004 - 2009
Ph.D. in Polymer Chemistry and Physics, Jun, 2009
Dissertation: *"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

Nanjing University, Nanjing, 2000 - 2004
B.S. in Chemistry, Jun, 2004
Thesis: *"Synthesis and Characterization of Amphiphilic Ligands and Its Complexes with Metal Ions"*
Advisor: Prof. Wei-Jiang He

Teaching Experience

- Polymer Physics (Core course for undergraduate students, 2014, 2017, 2018).
- Introduction to Polymeric Materials (for undergraduate students, 2016, 2017)

Research Grants

- Shanghai Pujiang Program (Principle Investigator, No. 18PJ1401200, 2018-2020)
- The Young Scientists Fund of the National Natural Science Foundation of China (NSFC) (Principle Investigator, No. 21004013, 2011-2013).

- The Shanghai Postdoctoral Scientific Program (Principle Investigator, No. 11R21411400, 2011-2011).
- The National Basic Research Program of China (No. 2011CB605701, 2013-2015).

Honors and Awards

- Visiting Scholar (China Scholar Council, No. 201406105018, 2014-2016)
- Dongkong Scholarship for Graduates (Peking University, 2008)
- Student Award of Merit (Peking University, 2008)
- Renming Scholarship (Nanjing University, 2000, 2001, 2002, 2003)

Professional Memberships and Activities

- Referee: *Polymer, Review of Scientific Instruments, Chinese Physics B*.

Computational Experience

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

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**, DOI: http://dx.doi.org/10.1021/acs.macromol.8b00349.
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**, Accepted. (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**, DOI: 10.1007/s10118-018-2100-4.
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)

* Full text of the listed publications are available at http://www.ngpy.org/publications.