Curriculum Vitae

Yi-Xin Liu

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Research Interests

- Static and dynamic properties of complex fluids, e.g. biological macromolecules (DNA, protein), polyelectrolytes, block copolymers, and polymer brushes in bulk or under geometrical confinements.
- Numerical algorithms for polymer field theory, molecular dynamics simulation, Monte-Carlo simulation, and phase field equations.
- Thin and ultrathin film polymer crystallization.

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

Research Experience

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

- Field-theoretic simulations of polymeric materials.

Lecturer, 2012 - present
Fudan University, Department of Macromolecular Science

- Chebyshev based self-consistent field theory (SCFT) studies of polymer brushes and polymers under confinements, focusing on the effect of surface affinity. The Chebyshev based SCFT algorithm is highly efficient on non-periodic boundary condition problems.
- Development of the polyorder project: a unified computing framework for performing polymer SCFT calculations.

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

- Developed high performance SCFT methods for studying the equilibrium phase separation structures of block copolymers and polyelectrolytes.
- Developed multigrid algorithms for solving Poisson-Boltzmann equations.
- Performed Monte-Carlo simulations on the nucleation and growth processes in thickening of monolayer PEO crystals in ultrathin films.

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

- Introduced the phase field simulation to study morphological evolution of monolayer poly(ethylene oxide) (PEO) crystals.
- Conducted experimental studies on the nucleation, growth, and thickening of monolayer PEO crystals in utralthin films using real-time atomic force microscopy (AFM).

Undergraduate Student, 2003 - 2004
Nanjing University, School of Chemistry and Chemical Engineering

- Synthesized three amphiphilic ligands and their complexes with Cu^{2+}.
- Computed surface properties of supported catalysts using Gaussian 98.

Research Grants

- The National Basic Research Program of China (2011CB605701, 2013-2015).
- The Shanghai Postdoctoral Scientific Program (11R21411400, 2011-2011).
- The Young Scientists Fund of the National Natural Science Foundation of China (NSFC) (21004013, 2011-2013).

Professional Memberships and Activities

- Member, American Physical Society (2013 - present)
- Referee, Polymer (2013 - present)

Honors and Awards

- Dongkong Scholarship for Graduates (Peking University, 2008)
- Student Award of Merit (Peking University, 2008)
- Renming Scholarship (Nanjing University, 2000, 2001, 2002, 2003)

Computatinal Experience

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

Publications

1. **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
2. **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
3. 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

4. **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
5. **Liu, Y. X.**; Chen, E. Q. "Polymer crystallization of ultrathin films on solid substrates." *Coordination Chemistry Reviews* **2010**, *254*, 1011–1037
6. 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
7. **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
8. 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
9. 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." *Frontiers of Chemistry in China* **2007**, *2*, 174–177
10. 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
11. 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
12. 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 Polymerica Sinica* **2006**, 553–556
13. 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 Polymerica Sinica* **2006**, 1125–1128

Postdoctoral Research Reports

1. **Liu, Y. X.** "Microphase Separation of Weakly Charged Polymers and Phase Transition Kinetics of Lamellar Crystal Monolayers.", Fudan University, Shanghai, **2012**

Presentations and Posters

1. **Liu, Y. X.** "Polymer Self-Consistent Field Theory in Bulk and under Confinement." *Talk at ASML Company*, **2014**
2. **Liu, Y. X.**; Zhang, H. D. "Exponential Time Differencing Methods for Numerical Self-Consistent Field Theory." *APS March Meeting*, **2014**
3. **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**
4. **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**
5. **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**
6. **Liu, Y. X.**; Chen, E. Q. "Isothermal Thickening of PEO Lamellar Crystals on Mica Surface." *Polymer Symposium of China*, Chengdu, **2007**

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