

# Curriculum Vitae

## Xuejin Li

Division of Applied Mathematics  
Brown University  
Providence, RI 02912

Tel: 401-935-8749  
E-mail: Xuejin.Li@brown.edu  
URL: <http://www.dam.brown.edu/people/xli/>

### EDUCATION

- June 2009 **PhD** in Chemistry and Physics of Polymers  
University of Science & Technology of China, P. R. China
- July 2004 **Bachelor of Economics** in Finance (dual degree)  
University of Science & Technology of China, P. R. China
- July 2004 **Bachelor of Engineering** in Polymer Material and Engineering  
University of Science & Technology of China, P. R. China

### RESEARCH INTERESTS

- Computational modeling and simulations of red blood cells in health and disease
- Multiscale modeling of soft matter and polymers
- Coarse-grained molecular dynamics of complex fluids at equilibrium and under shear

### RESEARCH EXPERIENCE

- Sept 2014 - present Assistant Professor (Research), Division of Applied Mathematics,  
Brown University
- Sept 2010 - Aug 2014 Postdoctoral Research Associate, Division of Applied Mathematics,  
Brown University
- Jun 2009 - May 2011 Research Associate, Department of Polymer Science & Engineering,  
University of Science & Technology of China
- Jul 2004 - May 2009 Research Assistant, Department of Polymer Science & Engineering,  
University of Science & Technology of China

### HONORS AND AWARDS

- Travel fund for *2013 NIMBioS Investigative Workshop on Modeling Blood Cell Interactions*
- Travel fund for *2011 AMS von Neumann Symposium on Multimodel and Multialgorithm Coupling for Multiscale Problems*
- Chinese Academy of Sciences (CAS) K. C. Wong Post-doctoral Fellowships in 2010
- Best Poster Award Winner at National Polymer Conference in 2009
- Chinese Academy of Sciences (CAS) Zhu-Li-Yuehua outstanding doctoral scholarship in 2009
- Outstanding post-graduate of University of Science and Technology of China in 2009
- Donggang post-graduate scholarship in academic year 2006-2007
- Excellent thesis award of University of Science and Technology of China in 2004
- Outstanding under-graduate student of *Xuxin* scholarship in academic year 2002-2003
- Outstanding under-graduate student scholarship in academic year 2001-2002

## PUBLICATIONS AND IMPACT

- **Researcher ID:** B-8559-2009
- **Publications:** 26 papers in refereed journals, including Macromolecules, Soft Matter (two most important journals in my field), PNAS, Chem Commun, Biophys J, PLOS Comput Biol, Nanoscale, J Chem Phys, J Phys Chem, Phys Chem Chem Phys, Philos T R Soc, and Polymer.
- **H-index:** 14 (Google Scholar), 12 (ISI Web of Science)
- **Total number of citations:** 461 (Google Scholar), 353 (ISI Web of Science)

## REFERRED JOURNAL PUBLICATIONS (\* indicates corresponding author)

1. **X. J. Li**, E. Du, H. Lei, M. Dao, S. Suresh, and G. E. Karniadakis\*. “Patient-specific modeling and predicting blood viscosity in sickle cell anemia”. *Interface Focus* **2015**, XX, submitted. (invited paper)
2. A. Yazdani<sup>§</sup>, **X. J. Li<sup>§</sup>**, and G. E. Karniadakis\*. “Dynamic and rheological properties of soft biological cell suspensions”. *Rheol. Acta* **2015**, 54, to appear. (<sup>§</sup> indicates these authors contributed equally to this work) (invited paper)
3. K. Lykov<sup>§</sup>, **X. J. Li<sup>§</sup>**, H. Lei, I. V. Pivkin\*, and G. E. Karniadakis\*. “Inflow/outflow boundary conditions for particle-based blood flow simulations: Application to arterial bifurcations and trees”. *PLOS Comput. Biol.* **2015**, 11, to appear. Doi: 10.1371/journal.pcbi.1004410. (<sup>§</sup> indicates these authors contributed equally to this work)
4. Z. Li, Y.-H. Tang, **X. J. Li**, and G. E. Karniadakis\*. “Mesoscale modeling of phase transition dynamics of thermoresponsive polymers”. *Chem. Commun.* **2015**, 51, 11038-11040.
5. **X. J. Li**, Y.-H. Tang, H. J. Liang\*, and G. E. Karniadakis\*. “Large-scale dissipative particle dynamics simulations of self-assembled amphiphilic systems”. *Chem. Commun.* **2014**, 50, 8306–8308.
6. **X. J. Li**, Z. L. Peng, H. Lei, M. Dao, and G. E. Karniadakis\*. “Probing red blood cell mechanics, rheology and dynamics with a two-component model”. *Philos. T. R. Soc. A.* **2014**, 372, 20130389.
7. Z. L. Peng, **X. J. Li**, I. V. Pivkin, M. Dao, G. E. Karniadakis and S. Suresh\*. “Lipid–bilayer and cytoskeletal interactions in a red blood cell”. *Proc. Natl. Acad. Sci. U.S.A.* **2013**, 110, 13356–13361.
8. **X. J. Li**\*. “Shape transformations of bilayer vesicles from amphiphilic block copolymers: A dissipative particle dynamics simulation study”. *Soft Matter* **2013**, 9, 11663–11670.
9. **X. J. Li**, P. V. Vlahovska, and G. E. Karniadakis\*. “Continuum- and particle-based modeling of shapes and dynamics of red blood cells in health and disease”. *Soft Matter* **2013**, 9, 28–37.
10. **X. J. Li**\*, I. V. Pivkin\*, and H. J. Liang\*. “Hydrodynamic effects on flow-induced polymer translocation through a microfluidic channel”. *Polymer* **2013**, 54, 4309–4317.
11. **X. J. Li**, B. Caswell, and G. E. Karniadakis\*. “Effect of chain chirality on the self-assembly of sickle hemoglobin”. *Biophys. J.* **2012**, 103, 1130–1140.
12. **X. J. Li**, A. S. Popel, and G. E. Karniadakis\*. “Blood-plasma separation in Y-shaped bifurcating microfluidic channels: A dissipative particle dynamics simulation study”. *Phys. Biol.* **2012**, 9, 026010(1–12).

13. **X. J. Li\***, X. L. Li, M. G. Deng, and H. J. Liang\*. “Effects of electrostatic interactions on the translocation of polymers through a narrow pore under different solvent conditions: A dissipative particle dynamics simulation study”. *Macromol. Theory Simul.* **2012**, *21*, 120-129. ([Most-accessed articles during the period of April 2012–March 2013](#))
14. J. Y. Guo, **X. J. Li\***, and H. J. Liang\*. “Dissipative particle dynamics simulations of fluid-driven polymer through a microchannel”. *Acta Polym. Sin.* **2012**, *2*, 160-167.
15. Y. F. Li, **X. J. Li**, Z. H. Li, and H. J. Gao\*. “Surface–structure–regulated penetration of nanoparticles across cell membrane”. *Nanoscale* **2012**, *4*, 3768-3775.
16. M. G. Deng, **X. J. Li**, H. J. Liang, B. Caswell, and G. E. Karniadakis\*. “Simulation and modeling of slip flow over surfaces grafted with polymer brushes and glycocalyx fibers”. *J. Fluid Mech.* **2012**, *711*, 192-211.
17. J. Y. Guo, **X. J. Li\***, Y. Liu, and H. J. Liang\*. “Flow-induced translocation of polymers through a fluidic channel: A dissipative particle dynamics simulation study”. *J. Chem. Phys.* **2011**, *134*, 134906(1-8).
18. P. T. He, **X. J. Li\***, M. G. Deng, T. Chen, and H. J. Liang\*. “Complex micelles from the self-assembly of coil-rod-coil amphiphilic triblock copolymers in selective solvents”. *Soft Matter* **2010**, *6*, 1539-1546.
19. P. T. He<sup>§</sup>, **X. J. Li<sup>§,\*</sup>**, D. Z. Kou, M. G. Deng, and H. J. Liang\*. “Complex micelles from the self-assembly of amphiphilic triblock copolymer in selective solvents”. *J. Chem. Phys.* **2010**, *132*, 204905(1-6). ([§ indicates these authors contributed equally to this work](#))
20. M. G. Deng, Y. Jiang, **X. J. Li\***, Y. Liu, L. Wang, and H. J. Liang\*. “Conformational behaviors of a charged-neutral star micelle in salt-free solution”. *Phys. Chem. Chem. Phys.* **2010**, *12*, 6135-6139.
21. **X. J. Li**, I. V. Pivkin, H. J. Liang\*, and G. E. Karniadakis\*. “Shape transformations of membrane vesicles from amphiphilic triblock copolymers: A dissipative particle dynamics simulation study”. *Macromolecules* **2009**, *42*, 3195-3200.
22. **X. J. Li**, J. Y. Guo, Y. Liu, and H. J. Liang\*. “Microphase separation of poly (styrene-*b*-isoprene) diblock copolymer: A dissipative particle dynamics simulation study”. *J. Chem. Phys.* **2009**, *130*, 074908(1-7).
23. **X. J. Li**, Y. Liu, L. Wang, M. G. Deng, and H. J. Liang\*. “Fusion and fission pathways of vesicles from amphiphilic triblock copolymers: A dissipative particle dynamics simulation study”. *Phys. Chem. Chem. Phys.* **2009**, *11*, 4051-4059.
24. **X. J. Li**, M. G. Deng, Y. Liu, and H. J. Liang\*. “Dissipative particle dynamics simulations of toroidal structure formations of amphiphilic triblock copolymers”. *J. Phys. Chem. B* **2008**, *112*, 14762-14765.
25. S. L. Rao, **X. J. Li**, and H. J. Liang\*. “Developing coarse-grained force fields for polystyrene with different chain lengths from atomistic simulation”. *Macromol. Res.* **2007**, *15*, 610-616.
26. **X. J. Li**, D. Z. Kou, S. L. Rao, and H. J. Liang\*. “Developing a coarse-grained force field for the diblock copolymer poly (styrene-*b*-butadiene) from atomistic simulation”. *J. Chem. Phys.* **2006**, *124*, 204909(1-7).
27. **X. J. Li**, X. J. Ma, L. Huang, and H. J. Liang\*. “Developing coarse-grained force fields for *cis*-poly (1,4-butadiene) from the atomistic simulation”. *Polymer* **2005**, *46*, 6507-6512.

## BOOK/CHAPTER

1. **X. J. Li**, Z. Li, X. Bian, M. G. Deng, C. H. Kim, Y.-H. Tang, Alireza Yazdani, and G. E. Karniadakis “Dissipative Particle Dynamics, Overview”. Essay in *Encyclopedia of Nanotechnology*. Springer, 2015, to appear.
2. X. H. He, **X. J. Li**, P. Chen, and H. J. Liang “Dynamics simulations of microphase separation in block copolymers”. Chapter in *Polymer morphology: principles, characterization, and processing*. John Wiley & Sons, Inc., 2015, Chapter 15.
3. **X. J. Li**, R. Huang, P. Chen, Y. Jiang, and H. J. Liang “Introduction to theoretical and modeling methods in polymer sciences”. Chapter in *Frontier aspects and development of polymer sciences*. Science Press, 2006, 375-395.

## REFERRED CONFERENCE PUBLICATIONS

1. **X. J. Li**, E. Du, H. Lei, M. Dao, and G. E. Karniadakis. “Patient-specific modeling and predicting blood viscosity in sickle cell anemia”. 2014 IMAG Multiscale Modeling Consortium Meeting, Bethesda, Maryland, United States, 2014. 09.
2. **X. J. Li**, H. Lei, E. Du, M. Dao, and G. E. Karniadakis. “Rheology of sickle cell anemia: Effects of heterogeneous RBC shapes”. 2014 SIAM Annual Meeting, Chicago, Illinois, United States, 2014. 07.
3. **X. J. Li**, K. Lykov, I. V. Pivkin, and G. E. Karniadakis. “Dissipative particle dynamics modeling of blood flow in arterial bifurcations”. 66th Annual Meeting of the APS Division of Fluid Dynamics, Pittsburgh, Pennsylvania, United States, 2013. 11.
4. **X. J. Li**, Z. L. Peng, M. Dao, and G. E. Karniadakis. “Probing red blood cell mechanics, rheology and dynamics with a two-component model”. Red Cell Club 2013, New York, New York, United States, 2013. 10.
5. **X. J. Li**, I. V. Pivkin, and G. E. Karniadakis. “Multiscale modeling of blood-plasma separation in bifurcations”. EMI2013 Conference, Evanston, Illinois, United States, 2013. 08.
6. **X. J. Li** and G. E. Karniadakis. “Morphology and chirality control self-assembly of sickle hemoglobin inside red blood cells”. 2013 NIMBioS Investigative Workshop—Modeling Blood Cell Interactions, Knoxville, Tennessee, United States, 2013. 06. ([Invited talk](#))
7. B. Caswell, H. Lei, **X. J. Li**, and G. E. Karniadakis. “Occlusion by cell-cell and cell-wall adhesion in sickle cell disease”. 2012 AIChE Annual Meeting, Pittsburgh, Pennsylvania, United States, 2012. 10.
8. **X. J. Li**, H. Lei, B. Caswell, and G. E. Karniadakis. “Morphology and chirality control self-assembly of sickle hemoglobin inside red blood cells”. APS March Meeting 2012, Boston, Massachusetts, United States, 2012. 03. ([Invited talk in Self-Assembling Structures Press Conference](#))
9. **X. J. Li**, A. S. Popel, and G. E. Karniadakis. “Multiscale modeling of blood-plasma separation in bifurcations”. 64<sup>th</sup> Annual Meeting of the APS Division of Fluid Dynamics, Baltimore, Maryland, United States, 2011. 11.
10. Y. F. Li, **X. J. Li**, and Z. H. Li. “Translocation of nanoparticles coated with amphiphilic molecules across a lipid bilayer membrane: A dissipative particle dynamics simulation study”. ASME 2011 International Mechanical Engineering Congress & Exposition (IMECE), Denver, Colorado, United States, 2011. 11.

11. **X. J. Li**, B. Caswell, and G. E. Karniadakis\*. "Self-assembly of sickle cell hemoglobin: A dissipative particle dynamics simulation study". The Society of Rheology: 83<sup>rd</sup> Annual Meeting, Cleveland, Ohio, United States, 2011. 10.
12. **X. J. Li**, P. T. He, and H. J. Liang. "Fluid-driven polymer translocation through a microchannel". 27<sup>th</sup> CCS (Chinese Chemical Society) Congress, Xiamen, P. R. China, 2010. 06. ([Invited talk in the session of Study of Theory, Analogy and Calculation on Polymer Sciences](#))
13. **X. J. Li** and H. J. Liang "Multiscale modeling and simulation of block copolymer". The National Polymer Conference in 2009 (NPC 2009), Tianjin, P. R. China, 2009. 08.
14. H. J. Liang and **X. J. Li**. "Shape transformations of membrane vesicles: A dissipative particle dynamics simulation study". The National Polymer Conference in 2009 (NPC 2009), Tianjin, P. R. China, 2009. 08.
15. **X. J. Li**, I. V. Pivkin, H. J. Liang, and G. E. Karniadakis. "Dissipative particle dynamics simulations of shape transformations of membrane vesicles from amphiphilic triblock copolymers". The International Conference on the Theory and Applications of Computational Chemistry in 2008 (TACC 2008), Shanghai, P. R. China, 2008. 09.
16. **X. J. Li**, M. G. Deng, P. Chen, and H. J. Liang. "Theoretical computation and simulations on self-assembly of block copolymers". 5<sup>th</sup> East-Asian Polymer Conference (EAPC-5), Shanghai, P. R. China, 2008. 06.
17. H. J. Liang, P. Chen, and **X. J. Li**. "Theory and simulation of the self-assembly of block copolymer". The National Polymer Conference in 2007 (NPC 2007), Chengdu, P. R. China, 2007. 10.
18. **X. J. Li**, S. L. Rao, D. Z. Kou, and H. J. Liang. "Developing a coarse-grained force field for polymer from atomistic simulation". 4<sup>th</sup> East-Asian Polymer Conference (EAPC-4), Tianjin, P. R. China, 2006. 05.

## PROFESSIONAL SERVICE

### Member:

- American Physical Society
- Chinese Chemical Society
- Institute of Physics

### Reviewer:

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| • ACS Nano   | • Macromolecules                              |
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| • Colloids and Surfaces A: Physicochemical and Engineering Aspects | • Colloids and Surfaces B: Biointerfaces      |
| • Drug Discovery Today: Disease Models                             | • Biomechanics and Modeling in Mechanobiology |
| • Macromolecular Theory and Simulations                            | • Materials Express                           |
| • Science China Chemistry  | • Theoretical Biology and Medical Modelling   |
| • Acta Physico-Chimica Sinica                                      | • Acta Polymerica Sinica                      |
| • Chinese Journal of Chemistry                                     | • Chinese Journal of Polymer Science          |
| • Chinese Journal of Chemical Physics                              | • Chemical Journal of Chinese Universities    |