

Curriculum Vitae

Xuejin Li

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EDUCATION

- June 2009 **Ph.D.** in Polymer Physics
University of Science & Technology of China, P. R. China
- July 2004 **B.Eng.** in Polymer Material and Engineering
B.Econ. in Financial Statistics (dual degree)
University of Science & Technology of China, P. R. China

RESEARCH EXPERIENCE

- Jun 2018 - *Hundred Talents Program* Professor, Department of Engineering Mechanics & Center for Soft Matter Science, Zhejiang University
- Jul 2017 - Jun 2018 Associate Professor (Research), Division of Applied Mathematics & Center for Fluid Mechanics, Turbulence and Computation, Brown University
- Sept 2014 - Jun 2017 Assistant Professor (Research), Division of Applied Mathematics, & Center for Fluid Mechanics, Turbulence and Computation, Brown University
- Sept 2012 - Aug 2014 Postdoctoral Research Associate, Division of Applied Mathematics
Brown University
- Jun 2009 - May 2012 Postdoctoral Research Associate, Department of Polymer Science & Engineering
University of Science & Technology of China

RESEARCH INTERESTS

- Soft matter physics
- Micro-/Nano-fluidics
- Cell biomechanics
- Molecullar hemorheology

HONORS, FELLOWSHIPS AND SCHOLARSHIPS

- Master of Arts *ad eundem* degree awarded at Brown University in 2018
- Hundred Talents Program of Zhejiang University in 2018
- DOE ASCR Leadership Computing Challenge (ALCC) Award in 2017–2018
- Travel fund for *2013 NIMBioS Investigative Workshop on Modeling Blood Cell Interactions*
- 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

GRANTS AND AWARDS

6. 2018.07–2024.06 Research Start-up Funds of Zhejiang University (“Hundred Talents Program”), “Multiscale modeling of hematological disorders”. Role: PI
5. 2017.07–2018.06 ASCR Leadership Computing Challenge (ALCC) Award (DOE), “Multiscale simulations of hematological disorders”, 46,000,000 supercomputing processor hours. Role: Co-PI (PI: George Em Karniadakis)
4. 2011.01–2013.12 National Natural Science Foundation of China, “Flow-induced translocation of polymers through a fluidic channel”. Role: PI
3. 2010.06–2012.05 Fundamental Research Funds for the Central Universities, “Dissipative particle dynamics simulations of shape transformations of polymeric vesicles under shear”. Role: PI
2. 2010.01–2011.12 K. C. Wong Education Foundation, Hong Kong, “Effect of hydrodynamic interaction on the translocation of polymers through a narrow channel”. Role: PI
1. 2009.07–2011.06 China Postdoctoral Science Foundation, “Numerical simulation of polymer/DNA translocation through a microfluidic channel”. Role: PI

PUBLICATIONS AND IMPACT

- **Researcher ID:** B-8559-2009
- **Publications:** 42 papers in refereed journals, including PNAS (3), Soft Matter (3), Biophys J (6), Macromolecules (2), Chem Commun (2), Nanoscale (2), J Fluid Mech (1), J Biomech (1), J Biomech Eng (1), Philos Trans R Soc (1), PLOS Comput Biol (3), Rheol Acta (1), Polymer (2), J Chem Phys (4), J Phys Chem B (2), Phys Chem Chem Phys (2), Phys Biol (1), and Interface Focus (1).
- **H-index:** 20 (Google Scholar); 18 (ISI Web of Science)
- **Total number of citations:** > 1180 (Google Scholar); > 840 (ISI Web of Science)

REFERRED JOURNAL PUBLICATIONS (*indicates corresponding author; § contributed equally)

43. S. Wang, H. Guo, **X. J. Li***, and Y. F. Li. “Penetration of nanoparticles across a lipid bilayer: Effects of particle stiffness and surface hydrophobicity”. *Nanoscale* **2019**, *11*, in revision.
42. Y. Deng, D. P. Papageorgiou, H.-Y. Chang, S. Z. Abidi, H. Lei, **X. J. Li***, M. Dao, and G. E. Karniadakis*. “Quantifying shear-induced deformation and detachment of individual adherent red blood cells in sickle cell disease”. *Biophys. J.* **2019**, *116*, 360-371.
41. H. Li§, L. Lu§, **X. J. Li**, P. Buffet, M. Dao*, G. E. Karniadakis*, and S. Suresh*. “Mechanics of diseased red blood cells in human spleen and consequences for hereditary blood disorders”. *Proc. Natl. Acad. Sci. U.S.A.* **2018**, *115*, 9574-9579.
40. D. P. Papageorgiou§, S. Z. Abidi§, H.-Y. Chang, **X. J. Li**, G. J. Kato, G. E. Karniadakis, M. Dao*, and S. Suresh*. “Simultaneous polymerization and adhesion under hypoxia in sickle cell anemia”. *Proc. Natl. Acad. Sci. U.S.A.* **2018**, *115*, 9473-9478. (*Highlighted by MIT News Report, The Bioscientist, and Xinhua News*)
39. H.-Y. Chang, A. Yazdani, **X. J. Li**, K. A. A. Douglas, C. Mantzoros, and G. E. Karniadakis*. “Quantifying platelet margination in diabetic blood flow”. *Biophys. J.* **2018**, *115*, 1371-1382. (*BJ Highlighted Article*)
38. L. Lu§, Y. X. Deng§, **X. J. Li**, H. Li, and G. E. Karniadakis*. “Quantifying understanding the twisted structure of amyloid fibrils via molecular simulations”. *J. Phys. Chem. B* **2018**, *122*, 11302-11310.
37. L. P. Chen, **X. J. Li**, Y. Zhang, T. Chen, M. He, X. Yin, S. Y. Xiao*, and H. J. Liang*. “Morphological and mechanical determinants of cellular uptake of deformable nanoparticles”. *Nanoscale* **2018**, *10*, 11969-11979.

36. H.-Y. Chang, **X. J. Li***, and G. E. Karniadakis*. “Modeling of biomechanics and biorheology of red blood cells in type-2 diabetes mellitus”. *Biophys. J.* **2017**, *113*, 481-490. (*BJ Highlighted Article*)
35. L. Lu, H. Li, X. Bian, **X. J. Li**, and G. E. Karniadakis*. “Mesoscopic adaptive resolution scheme toward understanding of interactions between sickle cell fibers”. *Biophys. J.* **2017**, *113*, 48-59. (*Cover Article*)
34. **X. J. Li**, E. Du, M. Dao*, S. Suresh, and G. E. Karniadakis*. “Patient-specific modeling of individual sickle cell behavior under transient hypoxia”. *PLOS Comput. Biol.* **2017**, *13*, e1005426. (*Highlighted on Biophysical Society Blog*)
33. **X. J. Li***, M. Dao, G. Lykotrafitis, and G. E. Karniadakis*. “Biomechanics and biorheology of red blood cells in sickle cell anemia”. *J. Biomech.* **2017**, *50*, 34-41. (*Quarterly Most-downloaded Articles, as of June 2017*)
32. **X. J. Li***, H. Li, H.-Y. Chang, G. Lykotrafitis, and G. E. Karniadakis*. “Computational biomechanics of human red blood cells in hematological disorders”. *ASME J. Biomech. Eng.* **2017**, *139*, 020804.
31. A. Blumers, Y.-H. Tang, Z. Li, **X. J. Li**, and G. E. Karniadakis*. “GPU-accelerated red blood cells simulations with transport dissipative particle dynamics”. *Comput. Phys. Commun.* **2017**, *217*, 171-179.
30. **X. J. Li**, E. Du, H. Lei, Y.-H. Tang, M. Dao, S. Suresh, and G. E. Karniadakis*. “Patient-specific modeling and predicting blood viscosity in sickle-cell anemia”. *Interface Focus* **2016**, *6*, 20150065.
29. H.-Y. Chang, **X. J. Li***, H. Li, and G. E. Karniadakis*. “MD/DPD multiscale framework for predicting morphology and stresses of red blood cells in health and disease”. *PLOS Comput. Biol.* **2016**, *12*, e1005173.
28. L. Lu, **X. J. Li***, P. G. Vekilov, and G. E. Karniadakis*. “Probing the twisted structure of sickle hemoglobin fibers via particle simulations”. *Biophys. J.* **2016**, *110*, 2085-2093. (*Feature Article*)
27. A. Yazdani[§], **X. J. Li[§]**, and G. E. Karniadakis*. “Dynamic and rheological properties of soft biological cell suspensions”. *Rheol. Acta* **2016**, *55*, 433-449.
26. Y.-H. Tang, Z. Li, **X. J. Li**, M. G. Deng, and G. E. Karniadakis*. “Non-equilibrium dynamics of vesicles and micelles by self-assembly of thermoresponsive block copolymers”. *Macromolecules* **2016**, *49*, 2895-2903.
25. K. Lykov[§], **X. J. Li[§]**, 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*, e1004410. (*Highlighted on LAMMPS homepage*)
24. 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.
23. **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.
22. **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. Trans. R. Soc. A.* **2014**, *372*, 20130389.
21. **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.
20. **X. J. Li***. “Shape transformations of bilayer vesicles from amphiphilic block copolymers: A dissipative particle dynamics simulation study”. *Soft Matter* **2013**, *9*, 11663-11670.
19. 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.

18. **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.
17. **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.
16. **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.
15. **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. (*Monthly and Yearly Most-accessed Articles, as of 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.
13. 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.
12. 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.
11. J. 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.
10. 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.
9. P. T. He[§], **X. J. Li^{§,*}**, 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.
8. 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.
7. **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.
6. **X. J. Li**, J. 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.
5. **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.
4. **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.
3. 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.
2. **X. J. Li**, D. Kou, S. 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. **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/ESSAY

8. **X. J. Li**, H. J. Lu, and Z. L. Peng. “Continuum- and particle-based modeling of human red blood cells”. Chapter in *Handbook of Materials Modeling (Vol. 2)*. Springer, 2018. Doi: 10.1007/978-3-319-50257-1_63-1.
7. **X. J. Li** and H. Lei. “Multiscale modeling of sickle cell anemia”. Chapter in *Handbook of Materials Modeling (Vol. 2)*. Springer, 2018. Doi: 10.1007/978-3-319-50257-1_67-1.
6. H. J. Liang, **X. J. Li**, and X. H. He. “Macromolecular Self-Assembling Systems: Theory and Simulation”. Chapter in *Emerging Trends in Macromolecular Self-Assembly*. China Science Publishing & Media Ltd., 2018, 75-103.
5. Z. Li, X. Bian, **X. J. Li**, M. Deng, Y.-H. Tang, B. Caswell, and G. E. Karniadakis. “Dissipative Particle Dynamics: Foundation, Evolution, Implementation, and Applications”. Chapter in *Particles in Flows*. Birkhauser/Springer, 2017, 255-326.
4. **X. J. Li** and G. E. Karniadakis. “*In-silico* medicine: multiscale modeling of hematological disorders”. *SIAM News* 2017, 50, online.¹
3. **X. J. Li**, Z. Li, X. Bian, M. G. Deng, C. H. Kim, Y.-H. Tang, A. Yazdani, and G. E. Karniadakis. “Dissipative Particle Dynamics, Overview”. Essay in *Encyclopedia of Nanotechnology*. Springer, 2016, 793–800.
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., 2016, 283-298.
1. **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*. China Science Publishing & Media Ltd., 2006, 375-395.

REFERRED CONFERENCE PUBLICATIONS

20. **X. J. Li**, Y. Deng, E. Du, L. Lu, M. Dao, J. M. Higgins, and G. E. Karniadakis. “Multiscale modeling of sickle cell disease”. 2018 NIH IMAG Futures Meeting – Moving Forward with the MSM Consortium, Bethesda, 2018. 03.
19. **X. J. Li**, E. Du, L. Lu, M. Dao, J. M. Higgins, and G. E. Karniadakis. “Patient-specific modeling of biomechanics and biorheology of red blood cells in sickle cell anemia”. 2017 NIH IMAG 10th Anniversary Multiscale Modeling Consortium Meeting, Bethesda, 2017. 03.
18. **X. J. Li**, M. Dao, J. M. Higgins, and G. E. Karniadakis. “Patient-specific modeling of individual sickle cell behavior under hypoxic conditions”. 2016 Red Cell Club Meeting, Manhasset, 2016. 10.
17. **X. J. Li**, E. Du, Z. Li, Y.-H. Tang, L. Lu, M. Dao, and G. E. Karniadakis. “Patient-specific modeling and analysis of dynamic behavior of individual sickle red blood cells under hypoxic conditions”. 68th Annual Meeting of the APS Division of Fluid Dynamics, Boston, 2015. 11.
16. **X. J. Li**, M. Dao, and G. E. Karniadakis. “Direct observation of individual sickle cell behavior under transient hypoxia”. 2015 IMAG Multiscale Modeling Consortium Meeting, Bethesda, 2015. 09.
15. **X. J. Li**, E. Du, M. Dao, and G. E. Karniadakis. “Patient-specific prediction of blood viscosity in sickle cell anemia”. 2014 IMAG Multiscale Modeling Consortium Meeting, Bethesda, 2014. 09.
14. **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, 2014. 07.
13. **X. J. Li**, K. Lykov, I. V. Pivkin, and G. E. Karniadakis. “Mesoscopic modeling of blood flow in arterial bifurcations”. 66th Annual Meeting of the APS Division of Fluid Dynamics, Pittsburgh, 2013. 11.

¹<https://sinews.siam.org/Details-Page/in-silico-medicine-multiscale-modeling-of-hematological-disorders>.

12. **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, 2013. 10. ([Invited talk](#))
11. **X. J. Li**, I. V. Pivkin, and G. E. Karniadakis. "Multiscale modeling of blood-plasma separation in bifurcations". Engineering Mechanics Institute Conference 2013, Evanston, 2013. 08.
10. **X. J. Li**, B. Caswell, and G. E. Karniadakis. "Morphology and chirality control self-assembly of sickle hemoglobin inside red blood cells". SES 50th Annual Technical Meeting, Providence, 2013. 07.
9. **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, 2013. 06. ([Invited talk](#))
8. 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, 2012. 10.
7. **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, 2012. 03. ([Invited talk in Self-Assembling Structures Press Conference](#))
6. **X. J. Li**, A. S. Popel, and G. E. Karniadakis. "Multiscale modeling of blood-plasma separation in bifurcations". 64th Annual Meeting of the APS Division of Fluid Dynamics, Baltimore, 2011. 11.
5. **X. J. Li**, B. Caswell, and G. E. Karniadakis*. "Mesoscopic modeling of the self-assembly of sickle cell hemoglobin". 83rd Annual Meeting of the Society of Rheology, Cleveland, 2011. 10.
4. **X. J. Li**, P. T. He, and H. J. Liang. "Fluid-driven polymer translocation through a microchannel". 27th CCS (Chinese Chemical Society) Congress, Xiamen, P. R. China, 2010. 06. ([Invited talk in the session of Study of Theory, Analogism and Calculation on Polymer Sciences](#))
3. **X. J. Li** and H. J. Liang "Multiscale modeling and simulation of block copolymer". The National Polymer Conference in 2009 (NPC 2009), Tianjin, China, 2009. 08.
2. **X. J. Li**, M. G. Deng, and H. J. Liang. "Theoretical computation and simulations on self-assembly of block copolymers". 5th East-Asian Polymer Conference (EAPC-5), Shanghai, China, 2008. 06.
1. **X. J. Li**, S. L. Rao, D. Z. Kou, and H. J. Liang. "Developing a coarse-grained force field for polymer from atomistic simulation". 4th East-Asian Polymer Conference (EAPC-4), Tianjin, China, 2006. 05.

PROFESSIONAL SERVICE

Member:

- American Physical Society
- Institute of Physics
- Chinese Chemical Society
- Chinese Society of Theoretical and Applied Mechanics

Reviewer/Panelist for Research Proposals Submitted to:

- National Institutes of Health (NIH)
- The Royal Society
- Swiss National Supercomputing Centre (CSCS)

Advisory Board:

- Review Editor for Frontiers in Physics
- International Advisory Committee for ICASET-17

Reviewer for:

- ACS Nano
- Soft Matter
- Journal of Biomechanics
- Journal of Computational Physics
- Physics of Fluids
- Biomicrofluidics
- Journal of Chemical Physics
- Science China Chemistry
- WIREs Systems Biology and Medicine
- Colloids and Surfaces A: Physicochemical and Engineering Aspects
- Drug Discovery Today: Disease Models
- International Journal for Numerical Methods in Fluids
- Molecular Simulation
- Materials Express
- Applied Mathematics and Mechanics
- Journal of Pain Research
- Acta Physico-Chimica Sinica
- Chinese Journal of Chemistry
- Chinese Journal of Chemical Physics
- Biophysical Journal
- Macromolecules
- Physical Review E
- Applied Physics Letters
- SIAM Journal on Scientific Computing
- IEEE Transactions on Nanotechnology
- Biomechanics & Modeling in Mechanobiology
- Polymer
- Science China Physics, Mechanics and Astronomy
- Colloids and Surfaces B: Biointerfaces
- International Journal of Numerical Methods for Heat and Fluid Flow
- International Journal for Numerical Methods in Biomedical Engineering
- Theoretical Biology and Medical Modelling
- Macromolecular Theory and Simulations
- PLOS One
- Sensors
- Micromachines
- Chinese Journal of Polymer Science
- Chemical Journal of Chinese Universities