

# Dejun Lin

## Curriculum Vitae

Department of Genome Sciences  
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## Education

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- **University of Rochester Medical Center** **Rochester, NY**  
*Ph.D. in Biophysics* 2013–2015
- **University of Rochester Medical Center** **Rochester, NY**  
*M.S. in Biophysics* 2010–2013
- **Nankai University** **Tianjin, China**  
*B.S. in Biological Sciences* 2006–2010

## Research Experience

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### Postdoctoral Research.....

**University of Washington** **Seattle, WA**  
*Advisors: William Noble and Cole Trapnell* 2016 – current

- **Design, validate and apply computational methods for interpreting single-cell Hi-C and RNA-seq data to better understand the relationship between genome 3D architecture and gene expression**

### Graduate Research.....

**University of Rochester Medical Center** **Rochester, NY**  
*Advisor: Alan Grossfield* 2010 – 2015

- **Determine the thermodynamics of antimicrobial lipopeptides' interaction with membranes via computer simulation and free energy calculation**  
- Methods: *nonlinear system dynamics; solve partial differential equations; statistical sampling; data mining*
- **Parametrize a coarse-grained force field based on Gay-Berne potentials and electric multipoles**  
- Methods: *quantum mechanics; machine learning*
- **Develop a novel algorithm to evaluate electric multipole interaction energy and gradients**  
- Methods: *linear algebra; tensor calculus; Fourier analysis*

### Undergraduate Research.....

**Nankai University** **Tianjin, China**  
*Tianjin Key Laboratory of Protein Science* 2009 – 2010

- **Solve the X-ray crystal structure of gentisate 1,2-dioxygenase from *Silicibacter pomeroyi* (GDOsp) bound to its substrate**

**Nankai University** **Tianjin, China**  
*Laboratory of Plant Molecular Biology* 2008 – 2009

- Improve the biochemical production of Vinblastine in *Catharanthus roseus* via plant tissue engineering

## Computational Skills

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### Software Developed.....

- **Generalized weighted histogram analysis method:** A C++11 template library for calculating free energy profile from various enhanced sampling schemes, <https://github.com/dejunlin/gwham>
- **Cartesian tensor-based generalized electric multipole interaction:** A C++11 template library for evaluating electric multipole interaction energy and gradients, <https://github.com/dejunlin/emp>
- **Contact-based reaction coordinate in umbrella sampling:** An extension to GROMACS 4.6.3 with OpenMPI parallelization (in house)
- **Gay Berne-Electric Multipole coarse grained force field:** An extension to LAMMPS (in house)
- **Improving the Distributed Replica Sampling software suite:** An extension to the original software package (in house)

### Programming Language.....

- I'm fluent in template meta-programming and object-oriented programming in C++. I have done a lot of scripting using Perl and Python. I'm also familiar with C and Fortran.

### Programming Environment.....

- I'm proficient at programming on Linux. I have experience with programming on Windows using MS Visual Studio. I'm fluent in using various GNU Vim-based IDE. I have experience with code analysis using Valgrind and code debugging using GDB. I'm familiar with version control tools such as Git and SVN.

### High Performance Computing.....

- I'm fluent in using message-passing or shared-memory based parallelization. I'm also familiar with vectorization using SSE and AVX intrinsics.

### Distributed Computing.....

- I'm familiar with socket and network programming. I have experience with developing API for cross-platform communication and distributed computing to achieve massive parallelization and enhanced sampling in molecular dynamics simulations.

## Publications

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1. **Dejun Lin**, Alan Grossfield *Coarsed-grained membrane force field based on Gay-Berne potential and electric multipoles*. In: *Many-Body Effects and Electrostatics in Biomolecules*. Ed. by Qiang Cui, Markus Meuwly, Pengyu Ren. in press. Pan Stanford Publishing. Chap. 14.
2. **Dejun Lin** *Generalized and efficient algorithm for computing multipole energies and gradients based on Cartesian tensors*. *J. Chem. Phys.* 143 (2015): 14115.
3. **Dejun Lin**, Alan Grossfield *Thermodynamics of Micelle Formation and Membrane Fusion Modulate Antimicrobial Lipopeptide Activity*. *Biophys. J.* 109 (2015): 750–759. **Recommended by the editor in *New and Notable of Biophys. J.* and announced in *EurekAlert! Science News*.**
4. **Dejun Lin**, Alan Grossfield *Thermodynamics of Antimicrobial Lipopeptide Binding to Membranes: Origins of Affinity and Selectivity*. *Biophys. J.* 107 (2014): 1862–1872.

5. Joshua N. Horn, Jesse D. Sengillo, **Dejun Lin**, Tod D. Romo, Alan Grossfield *Characterization of a potent antimicrobial lipopeptide via coarse-grained molecular dynamics*. *Biochim. Biophys. Acta, Biomembr.* 1818 (Feb. 2012): 212–218.
6. Wenzheng Zhang, Wei Peng, Mingzhuo Zhao, **Dejun Lin**, Zonghao Zeng, Weihong Zhou, Mark Bartlam *Expression, purification and preliminary crystallographic analysis of human thyroid hormone responsive protein*. *Acta Crystallogr Sect F Struct Biol Cryst Commun* 67 (Aug. 2011): 941–946.

## Conference Presentations

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1. **Dejun Lin**, Alan Grossfield *Thermodynamics govern the mechanism of antimicrobial lipopeptides: insights from coarse-grained molecular dynamics simulations*. In: **59th Annual Biophysical Society Meeting**. Baltimore, MD, USA, Feb. 7–11, 2015.
2. **Dejun Lin**, Alan Grossfield *Investigation of the mechanism of antimicrobial lipopeptides using coarse-grained molecular dynamics simulations*. In: **58th Annual Biophysical Society Meeting**. San Francisco, CA, USA, Feb. 15–19, 2014.
3. **Dejun Lin**, Alan Grossfield *Investigation of the mechanism of antimicrobial lipopeptides using coarse-grained molecular dynamics simulations*. In: **Computational Chemistry Gordon Research Conference**. Mount Snow, VT, USA, July 19–25, 2014.
4. **Dejun Lin**, Joshua Horn, Zhen Xia, Pengyu Ren, Alan Grossfield *Investigation of the mechanism of antimicrobial lipopeptides using coarse-grained molecular dynamics simulations*. In: **57th Annual Biophysical Society Meeting**. Philadelphia, PA, USA, Feb. 2–6, 2013.
5. **Dejun Lin**, Joshua Horn, Alan Grossfield *Estimating the free energy to bind a potent antimicrobial lipopeptide to a model membrane bilayer*. In: **56th Annual Biophysical Society Meeting**. San Diego, CA, USA, Feb. 25–29, 2012.

## Honor and Awards

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### Presentation Awards.....

- Student Seminar Award, 2014 fall and 2012 spring
- Elena Gilde Grossfield presentation award, 2013
- Graduate Student Society poster competition award, 2014

### Fellowship.....

- The Elon Huntington Hooker Graduate Fellowship, 2014
- The Leon L. Miller Graduate Fellowship, 2011
- Second-class Scholarship of Nankai University in 2009, 2008 and 2007
- The Freshmen Scholarship of Nankai University in 2006

### Travel Grants.....

- Neuman Travel Award, 2014, 2013, 2012

### Others.....

- Wallace O. Fenn Award for excellent thesis research, 2016