

Curriculum Vitae

Lin Li

Department of Physics and Astronomy,
Clemson University
SC, United States, 29631
Email: lli5@clemson.edu
Phone: 1-636-364-8518

Research and work experience:

- 2016-now: **Research Assistant Professor**, Clemson University
- 2013-2016: **Research Associate**, Clemson University
Advisor: Prof. Emil Alexov
- 2011-2013: **Postdoctoral Researcher**, Clemson University
Advisor: Prof. Emil Alexov
- 2010-2011: **Research Assistant**, Huazhong University of Science and Technology
Advisor: Prof. Yi Xiao

Education:

- 2005-2011 **Ph.D. (Biophysics)**, Huazhong University of Science and Technology
 - 2001-2005 **B.S. (Applied Physics)**, Huazhong University of Science and Technology
-

Research experience:

DelPhi Development

I have developed many algorithms and tools in DelPhi C++ package, which is an Object-Oriented program that computes the electrostatic potential of proteins, RNAs, DNAs and nano objects. Once the potential is calculated, the corresponding electrostatic force and energy components are also delivered. Since 2011, DelPhi has been downloaded and used by over 3,000 research groups around the world. <http://compbio.clemson.edu/delphi>

Large-Scale Simulation Package

I have developed the multi-scale approach, which use Monte Carlo algorithm to model the binding process between large and small biological objects. Examples include but are not limited to motor domain binding to microtubules, protein binding to viruses, protein binding to a membrane and many others. I developed a novel algorithm that first calculates electrostatic energy at a coarse-grained resolution in the entire system. Then it transfers the information from the entire environment to focused local regions and calculates the electrostatic energies at finer resolution.

Inhomogeneous dielectric model

I have developed an inhomogeneous dielectric model for electrostatic energy calculations, which provides better physical ground in modeling biological macromolecules. The model has been proved successful in the areas of electrostatic potential calculations, solvation energy calculations, pKa predictions and binding energy calculations.

MEMPOT

I developed the Membrane Potential (MEMPOT) tool and implemented it into DelPhi program. Using this MEMPOT tool, one can easily calculate the electrostatic potential distribution across a membrane.

ASPDock

I have developed a docking algorithm (ASPDock) to calculate binding free energy of protein-protein and protein-DNA complexes, which improves the accuracy of predictions. Comparisons with other state-of-the-art docking algorithms showed that ASP score indeed gives higher success rate than the pure shape complementarity score of FTDock.

SRM

I also developed a Softly Restricting Method (SRM), which utilizes the unreliable binding site information to enhance success rate of protein-protein and protein-DNA docking. It only reduces hit count number and success rate slightly if the predicted information is completely wrong. However, when the predicted information is correct or partially correct, SRM increases the hit count number and success rate significantly.

CAPRI

Using ASPDock and Softly Restricting Method, my team has participated in two rounds of Critical Assessment of PRediction of Interactions (CAPRI). We got high-quality hits for T40 and T41 and the best LRMSD were 2.35 Å and 1.41 Å, respectively. (ranking 6th in 40+ teams)

Teaching experience:

2013-now: Instructor of **Computational Physics**, Physics Department at Clemson University

2007-2011: Lecture of **Digital Photography**, Wuhan Media and Communications College at Huazhong Normal University

2005-2006: Teaching Assistant of **Physics Laboratory**, Physics Department of Huazhong University of Science and Technology

Selected Awards:

- 2016: FASEB (Federation of American Societies for Experimental Biology) MARC Travel Award
- 2011: National Scholarship from Ministry of Education of the P.R. China (top 0.2% in China)
- 2005-2009: Excellent Leader of Student Groups in University in HUST (4 Consecutive)

years)

- 2002: National Scholarship from Ministry of Education of the P.R. China (top 0.2% in China)
 - 2003-2004: Individual Scholarship in HUST (2 Consecutive years)
 - 2002: The First Prize Scholarship in HUST
-

Intellectual properties:

IP. Tech ID: 2016-0036; IR: 626401-15-0045; **Multi-scale simulation package (MSSP)**; Grant Sponsor: GM093937, National Institutes of Health; PI: E. Alexov; Disclosure date: 2016-03-26.

IP. Tech ID: 2013-021 1; IR: 626401-12-0017; **Gaussian Dielectric Function in DelPhi**; Grant Sponsor: GM093937, National Institutes of Health; PI: E. Alexov; Disclosure date: 2012-08-14.

IP. Tech ID: 2013-018; IR: 1626401-12-0015; **Algorithms and Computer Code for Parallel Computing of Electrostatics in Systems Made of Biological Macromolecules and Objects**; Grant support: GM093937, National Institutes of Health; PI; E Alexov; Disclosure date: 2012-08-13.

Editor:

I work as an editor for several journals, such as: *Journal of Scientific and Industrial Metrology*, *Aperito Journal of Computer Science and Biology*, *Journal of Chemical Biology & Therapeutics*, *Journal of Metrology*, *Insight Medical Publishing Journals*, etc.

Reviewer:

I am a reviewer for many journals, such as: *Plos One*, *Journal of Physical Chemistry*, *Proteins*, *European Biophysics Journal*, *Journal of Molecular Biology Research*, *Journal of Theoretical and Computational Chemistry*, *Computational and Mathematical Modeling in Medicine*, *Journal of Molecular Graphics and Modelling*, *Physical Chemistry Chemical Physics*, etc.

Publications and Presentations:

Selected Publications: (citation: 450+; h-index: 11)

1. **Lin Li**, Joshua Alper, and Emil Alexov. **Cytoplasmic dynein binding, run length, and velocity are guided by long-range electrostatic interactions**, *Scientific Reports* 6 (2016).
2. **Lin Li**, Joshua Alper, and Emil Alexov. **Multiscale method for modeling binding phenomena involving large objects: application to kinesin motor domains motion along microtubules**, *Scientific Reports*, 6 (2016): 23249.

3. Arghya Chakavorty, Lin Li, and Emil Alexov. **Electrostatic component of binding energy: Interpreting predictions from poisson–boltzmann equation and modeling protocols.** *Journal of Computational Chemistry* 37.28 (2016): 2495-2507.
4. Lin Wang, Lin Li, and Emil Alexov. **pKa Predictions for Proteins, RNAs and DNAs with the Gaussian Dielectric Function Using DelPhiPKa.** *Proteins: Structure, Function, and Bioinformatics* 83.12 (2015): 2186-2197.
5. Lin Li, Lin Wang, Emil Alexov, **On the energy components governing molecular recognition in the framework of continuum approaches,** *Frontiers in Molecular Biosciences* 2 (2015): 5.
6. Tugba G. Kucukkal, Marharyta Petukh, Lin Li, and Emil Alexov, **Structural and physico-chemical effects of disease and non-disease nsSNPs on proteins,** *Current opinion in structural biology* 32 (2015): 18-24.
7. Lin Li, Chuan Li, Emil Alexov, **On the Modeling of Polar Component of Solvation Energy Using Smooth Gaussian-Based Dielectric Function,** *Journal of Theoretical and Computational Chemistry*, 2014.
8. Roberta Dias^{\$}, Lin Li^{\$}, Thereza A. Soares and Emil Alexov, **Modeling the Electrostatic Potential of Asymmetric Lipopolysaccharide Membranes: The MEMPOT Algorithm Implemented in DelPhi,** *Journal of computational chemistry* (2014). (^{\$} contributed equally)
9. Praveen Nedumpully-Govindan, Lin Li, Emil G Alexov, Mark A Blenner, Feng Ding, **Structural and energetic determinants of tyrosylprotein sulfotransferase sulfation specificity,** *Bioinformatics*, 2014
10. Lin Li, Chuan Li, Zhe Zhang, Emil Alexov, **On the Dielectric "Constant" of Proteins: Smooth Dielectric Function for Macromolecular Modeling and Its Implementation in DelPhi,** *J Chem Theory Comput.* 2013 Apr 9;9(4):2126-2136.
11. Lin Li, Yanzhao Huang, and Yi Xiao, **How to Use Not-Always-Reliable Binding Site Information in Protein-Protein Docking Prediction,** *PLoS one* 8.10 (2013)
12. Chuan Li, Lin Li, Marharyta Petukh, Emil Alexov, **Progress in developing Poisson-Boltzmann equation solvers,** *Molecular Based Mathematical Biology.* Volume 1, Pages 42-62
13. Chuan Li, Marharyta Petukh, Lin Li, Emil Alexov, **Continuous development of schemes for parallel computing of the electrostatics in biological systems: Implementation in DelPhi,** *J Comput Chem.* 2013 Jun 4. doi: 10.1002/jcc.23340. [Epub ahead of print] PMID: 23733490
14. Huang, Yangyu, Shiyong Liu, Dachuan Guo, Lin Li, and Yi Xiao. **A novel protocol for three-dimensional structure prediction of RNA-protein complexes,** *Scientific reports* 3 (2013).
15. Lin Li, Li C, Sarkar S, Zhang J, Witham S, Zhang Z, Wang L, Smith N, Petukh M, Alexov E.* **DelPhi: a comprehensive suite for DelPhi software and associated resources,** *BMC Biophys,* (2012) May14;4(1):9.
16. Smith N, Campbell B, Li L, Li C, Alexov E., **Protein Nano-Object Integrator (ProNOI) for generating atomic style objects for molecular modeling,** *BMC Struct Biol.* 2012 Dec 5;12:31. doi:10.1186/1472-6807-12-31.
17. Chuan Li, Lin Li, Marharyta Petukh and Emil Alexov; **Progress in developing Poisson-**

Boltzmann equation solvers, Molecular Based Mathematical Biology. Volume 1, Pages 42-62.

18. Petukh M, Zhenirovskyy M, Li C, **Li L**, Wang L, Alexov E, **Predicting nonspecific ion binding using Delphi**, Biophys J. 2012 Jun 20, 102(12)
19. Chuan Li, **Lin Li**, Jie Zhang, Alexov E.*, **Highly efficient and exact method for parallelization of grid-based algorithms and its implementation in DelPhi**, J Comput Chem. (2012)
20. Lin Wang, Shawn Witham, Zhe Zhang, **Lin Li**, Michael Hodsdon and Emil Alexov*, **In silico investigation of pH-dependence of prolactin and human growth hormone binding to human prolactin receptor**, Comm. Comp. Phys., (2013), 13, 207-222
21. Nicholas Smith, Subhra Sarkar, Shawn Witham, Jie Zhang, **Lin Li**, Chuan Li and Emil Alexov*, **DelPhi Web Server v2: Incorporating atomic-style geometrical figures into the computational protocol**, Bioinformatics (2012), 28(12):1655-7.
22. **Lin Li**, Dachuan Guo, Yangyu Huang, Shiyong Liu, Yi Xiao*, **ASPDock: protein-protein docking algorithm using atomic solvation parameters model**, BMC Bioinformatics, 2011, 12(1): 36.
23. Changjun Chen, **Lin Li** and Yi Xiao*, **Identification of key residues in proteins by using their physical characters**. Physical Review E. 2006, 73(4): 41926.
24. Changjun Chen, **Lin Li** and Yi Xiao*, **All-Atom Contact Potential Approach to Protein Thermostability Analysis**, Biopolymers, 2007, 85(1): 28.

Presentations:

1. (invited talk) **Lin Li**, Emil Alexov, **Electrostatic interactions play important roles in kinesin proceeding on microtubule**, Mathematical Biosciences Institute workshop: Multiple Faces of Biomolecular Electrostatics, October 12-16, 2015, Columbus, OH, US.
2. (invited talk) **Lin Li**, Chuan Li, Emil Alexov, **Smooth dielectric function for modeling electrostatics in biological macromolecules**, 246th ACS National Meeting, September 8-12, 2013, Indianapolis, IN, US.
3. **Lin Li**, Emil Alexov, **Electrostatic interactions play important role in dynein's motion along microtubule in the cell**, CUPDA Postdoc Seminar, May 03, 2016, Clemson, SC.
4. (invited talk) **Lin Li**, Chuan Li and Emil Alexov, **Implementing smooth dielectric function to pKa predictions and other applications**, Protein Electrostatics Meeting: July 8-12, 2013, Telluride Science Research Center, Telluride, CO, US.
5. **Lin Li**, Chuan Li, and Emil Alexov, **Modeling proteins and small molecules with inhomogeneous dielectric function: Implementation in DelPhi**, Biophysical Society 57th Annual Meeting: February 2-6, 2013, Philadelphia, PA, US.
6. **Lin Li**, Chuan Li, Zhe Zhang, Emil Alexov, **Modeling bio-molecules with Gaussian smooth dielectric function**. Clemson Bioseminar, January 29, 2013, Clemson University, Clemson, SC, US.
7. (invited talk) **Lin Li**, Lin Wang, Chuan Li, and Emil Alexov, **The effect of non-uniform protein dielectric constant on the electrostatic energy calculations**, 244th ACS National Meeting, August 19-23, 2012, Philadelphia, PA, US.
8. **Lin Li**, **Protein-protein interactions and docking algorithms**, Clemson Bio-seminar,

September 9 2011, Clemson University, Clemson, SC, US.

9. **Lin Li**, Ying Chen and Yi Xiao, ***Using ASP model in a docking algorithm (Presentation)***, (HUST) Physics Department Seminar, January 12-13, 2009, Wuhan, China.

Posters:

1. **Lin Li**, Joshua Alper, Emil Alexov, ***long-range electrostatic interactions play important roles of dyneins' motion on microtubule***, Muscle & Molecular Motors, Gordon Research Conference, Mount Snow, West Dover, VT, July 17-22, 2016.
2. **Lin Li**, Joshua Alper, Emil Alexov, ***Electrostatics involvement in dyneins' binding and stepping on microtubule***, The Triangle Cytoskeleton Meeting 2016, Saxapahaw NC, September 12, 2016.
3. **Lin Li**, Joshua Alper, Emil Alexov, ***Electrostatic interaction is a key factor for dynein walking along microtubule***, 2016 Clemson University Research Symposium, Clemson, SC, May 03, 2016
4. **Lin Li**, Lin Wang and Emil Alexov, ***Predicting structured water molecules by combined energy calculations and geometrical considerations***, Symposium for Introduction to Research in Physics and Astronomy (SIRPA), BellSouth Auditorium, Clemson, SC, August 22, 2011
5. **Lin Li**, Dachuan Guo, Shiyong Liu and Yi Xiao, ***Protein-Protein Docking Algorithm Using ASP Model (Poster)***, Fourth CAPRI Evaluation Meeting, December 9-11, 2009, Barcelona, Spain.
6. **Lin Li**, Dachuan Guo and Yi Xiao, ***Computation of interactions between cannabinoid receptors and G-proteins (Poster)***, the 11th Chinese Conference on Biophysics, Guilin (China), July 12-16, 2009

References:

Prof. Emil Alexov,

Department of Physics and Astronomy

Clemson University

SC, U.S. 29634

Phone: 1-864-656-5307

Email: ealexov@clemson.edu

Prof. Guowei Wei,

Department of Mathematics

Department of Electrical & Computer Engineering

Adjunct Professor of Biochemistry & Molecular Biology

Michigan State University

D301 Wells Hall, 619 Red Cedar Road

East Lansing, MI 48824, USA

Phone: 517 353 4689