

# JIANING LI

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## PROFESSIONAL EXPERIENCE

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**Purdue University** **West Lafayette, IN**  
*Associate Professor of Medicinal Chemistry and Molecular Pharmacology* (2022–Present)  
Current research interests include:

- Creating new multiscale theory, methods, and models for rational drug and materials design;
- Developing machine learning approaches for high-throughput design of biologics & nanomedicines.

**Stanford University** **Palo Alto, CA**  
*Visiting Associate Professor in Electrical Engineering* (Summer 2022)

**The University of Vermont** **Burlington, VT**  
*Associate Professor of Chemistry* (2020–2022); *Assistant Professor of Chemistry* (2014–2020)

## EDUCATION

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**The University of Chicago** (August 2011–June 2014) **Chicago, IL**  
Postdoctoral Researcher

**Columbia University** (August 2006–August 2011) **New York, NY**  
**Ph.D.** in Chemical Physics, July 2011; **M. Phil.**, May 2010; **M.A.**, May 2007  
*Thesis:* Towards High-Resolution Computational Approaches for Structure-Based Drug Discovery

**University of Science and Technology of China** (September 2002–July 2006) **Hefei, China**  
**B.S.** in Chemical Physics, July 2006; Honors Thesis.

## RESEARCH EXPERIENCE

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**The University of Chicago, Department of Chemistry** (August 2011–June 2014) **Chicago, IL**  
*Postdoctoral Researcher*  
Advisor: Professor Gregory A. Voth

- Designed multiscale models of medically important proteins including GPCRs and kinases;
- Developed systematic and robust coarse-graining methods for membrane proteins.

**Columbia University, Department of Chemistry** (August 2006–August 2011) **New York, NY**  
*Graduate Research Assistant*  
Advisor: Professor Richard A. Friesner

- Developed the VSGB 2.0 energy model with near 100% success rate in predicting conformations of protein loop structures. One of the developers of the commercial software *Prime* of Schrödinger, *Inc.*;
- Invented IDSite (now the Schrödinger product *P450 SOM Prediction*), an accurate approach to predict drug metabolism mediated by human P450 enzymes, which is related to drug toxicity.

**Biomass and Clean Energy Laboratory** (May 2004–July 2006) **Hefei, China**  
*Undergraduate Research Assistant*  
Advisors: Professors Qingxiang Guo and Yao Fu

- Predicted acidity and bond dissociation enthalpies with Quantum Mechanics (QM).

## PAPERS IN PREPARATION/REVISION (\* = JL as a Corresponding Author)

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1. Remington, J. M.; Ferrell, J. B.; van Oort, C. M.; Sharafi, M.; Aboushousha, R.; Janssen-Heininger, Y.; Schneebeli, S. T.; Wargo M. J.; **Li, J.\*** “Molecular Modeling Improves Antimicrobial Peptide Design with Deep Learning” *Chem. Sci.* **2022**, Under Revision. ([bioRxiv](#))
2. McCarthy, D. R.; Remington, J. M.; Ferrell, J. B.; Schneebeli, S. T.; **Li, J.\*** “Bio-Nano Interactions between DNA Nanocages and Human Serum Albumin” *ACS Nano* **2022**, Resubmitted.
3. Villalba, N.; Sackheim, A. M.; Lawson, M.; Haines, L.; Chen, Y-L.; Sonkusare, S.; Ma, Y-T.; **Li, J.**; Majumdar, D.; Bouchard, B.; Boyson, J.; Poynter, M. E.; Nelson, M. T.; Freeman, K. “The Polyanionic Drug Suramin Neutralizes Histones and Prevents Endotheliopathy” *Am. J. Physiol.* **2022**, Under Revision.
4. Corteselli, E. M.; Sharafi, M.; MacPherson, M.; White, C.; Mauel, A.; van der Vliet; Anathy, V.; Schneebeli, S. T.; **Li, J.\***; Janssen-Heininger, Y. “Structural and Functional Fine Mapping of Cysteines in Mammalian Glutaredoxin Reveal a Hierarchy of Susceptibility to Oxidative Inactivation” *Nat. Comm.* **2022**, Under Revision.
5. Sharafi, M.; Scannell, M. J.; Woods, T. J.; Gray, D. L.; **Li, J.**; Schneebeli, S. T. “Magnolarenes -- A New Class of Macrocycles Capable of Exponential and Regiochemical Replication” *Org. Chem. Front.* **2022**, Under Revision.
6. Remington, J. M.; Ferrell, J. B.; Beckage, N.; **Li, J.\*** “Rapid Screening for GPCR Ligands Using Graph Convolutions and Deep Learning” *J. Chem. Inf. Model.* **2022**, Submitted.
7. Trinh, T.; Thompson, I.; Clark, F.; Remington, J. M.; **Li, J.\***; Einstein, M.; Soh, T. “A Modular Intramolecular Triplex Photo-Switching Motif that Enables Rapid and Reversible Control of Aptamer Binding Activity” *ACS Nano.* **2022**, Resubmitted.
8. Rafique, M. G.; Remington, J. M.; Clark, F.; Toader, V.; Perepichka, D. F.; **Li, J.\***; Sleiman, H. “Two-Dimensional Supramolecular Polymerization of DNA Amphiphiles Is Driven by Sequence-Dependent DNA-Chromophore Interactions” *Angew. Chem. Int. Ed.* **2022**, Under Revision.
9. Ferrell, J. B.; Zorman, M.; Remington, J. M.; Schneebeli, S. T.; **Li, J.\*** “Programmable Fluctuation of DNA Nanocages” *J. Phys. Chem. Lett.* **2022**, In Preparation.
10. Thapa, S.; Clark, F.; Zorman, M.; Schneebeli, S. T.; **Li, J.\*** “Benchmarking of Multiscale Models to Simulate Peptide Aggregation” *Phys. Chem. Chem. Phys.* **2022**, In Preparation.
11. Remington, J. M.; Ferrell, J. B.; Schneebeli, S. T.; **Li, J.\*** “Recovery of the Atomistic Protein Structure from the Coarse Grain Resolution with Machine Learning” *J. Chem. Theory Comput.* **2022**, In Preparation.
12. Mustafa, R.; Fitian, M.; Hamilton, N. B.; **Li, J.**; Silva, W. R.; Punihaole, D. “Molecular Insights into the Binding of Linear Polyethyleneimines and Single-stranded DNA Using Raman Spectroscopy: A Quantitative Approach” *J. Phys. Chem. B* **2022**, Under Review.
13. Murphy, K. E.; McKay, K. T.; Schenkelberg, M.; Sharafi, M.; Ivancic, M.; Li, J.; Schneebeli, S. T. “Helical Molecular Springs with Tunable Spring Constants” *Angew. Chem. Int. Ed.* **2022**, Under Revision.

## INDEPENDENT RESEARCH PUBLICATIONS (\* = JL as a Corresponding Author)

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1. McKay, K.; Hamilton, N.; Remington, J. M.; Schneebeli, S. T.; **Li, J.\*** “Essential Dynamics Ensemble Docking for Structure-Based GPCR Drug Discovery” *Front. Mol. Biosci.* **2022**, Accepted
2. **Li, J.\***; Remington, J. M.; Liao, C.; Parsons, R. L.; Schneebeli, S. T.; Braas, K. M.; May, V.; Brewer, M. “GPCR Intracellular Loops Regulation of beta-Arrestin-Mediated Endosomal Signaling Dynamics” *J. Mol. Neurosci.* **2022**, ASAP.
3. Remington, J. M.; Ferrell, J. B.; Schneebeli, S. T.; **Li, J.\*** “Concerted Rolling and Penetration of Peptides during Membrane Insertion” *J. Chem. Theory Comput.* **2022**, ASAP. ([arXiv](#))
4. Hamilton, N.; Remington, J. M.; Schneebeli, S. T.; **Li, J.\*** “Outcome-Based Redesign of Physical Chemistry Laboratories During the COVID-19 Pandemic” *J. Chem. Ed.* **2022**, 2, 639.
5. Ghalehgholabbehbahani, A.; Vestrheim, O.; Skinner, M.; **Li, J.**; Schneebeli, S. T. “Effect of Drying Temperature Regimes on the Quality of Vermont Grown Saffron (*Crocus sativus*)” *ACS Food Sci. Technol.* **2022**, 2, 206. ([Supplementary Cover](#))
6. van Oort, C. M.; Ferrell, J. B.; Remington, J. M.; Wshah, S.; **Li, J.\*** “AMPGAN v2: Machine Learning Guided Design of Antimicrobial Peptides” *J. Chem. Inf. Model.* **2021**, 61, 2198–2207. ([March Front Cover](#))
7. Zhao, X.; Hameed, U. F. S.; Kharchenko, V.; Liao, C.; Huser, F.; Remington, J. M.; Radhakrishnan, A. K.; Jaremko, M.; Jaremko, L.; Arold, S.; **Li, J.\*** “Molecular Basis for the Adaptive Evolution of Environment-sensing by H-NS Proteins” *eLife* **2021**, 10, e57467.
8. Zhao, X.; Remington, J. M.; Liao, C.; Schneebeli, S. T.; **Li, J.\*** “Molecular Basis of a Nucleoid-Structured Bacterial Protein Filament for Environment Sensing” *J. Phys. Chem. Lett.* **2021**, 12, 7878. ([August Supplementary Cover](#))
9. Dore, M. D.; Trinh, T.; Zorman, M.; de Rochambeau, D.; Xu, P.; Luo, X.; Remington, J. M.; Toader, V.; **Li, J.\***; Sleiman, H. F. “Thermosetting Supramolecular Polymerization of Compartmentalized DNA Fibers with Stereo-Sequence Control” *Chem* **2021**, 7, 2395–2414.
10. **Li, J.\***; McKay, K. T.; Remington, J. M.; Schneebeli, S. T. “A Computational Study of Cooperative Binding to Multiple SARS-CoV-2 Proteins” *Sci. Rep.* **2021**, 11, 16307.
11. Remington, J. M.; McKay, K.; Ferrell, J. B.; Schneebeli, S. T.; **Li, J.\*** “Enhanced Sampling Protocol to Elucidate Fusion Peptide Opening of SARS-CoV-2 Spike Protein” *Biophys. J.* **2021**, 120, 2848.
12. Liao, C.; Remington, J. M.; May, V.; **Li, J.\*** “Molecular Basis of Class B GPCR Selectivity for the Neuropeptides PACAP and VIP” *Front. Mol. Biosci.* **2021**, 644644. ([Invited Submission to Special Research Topic](#))
13. Jaynes, T. J.; Sharafi, M.; Campbell, J. P.; Becanegra, J.; McKay, K. T.; Little, K.; Brown, R. O.; Gray, G. L.; Woods, T. J.; **Li, J.**; Schneebeli, S. T. “Iterative Exponential Growth of Oxygen-linked Aromatic Polymers Driven by Nucleophilic Aromatic Substitution Reactions” *Front. Chem.* **2021**, 620017. ([Invited Submission to Special Research Topic](#))

14. Rajappan, S. C.; Vestrheim, O.; Sharafi, M.; **Li, J.**; Schneebeli, S. T. “Carbonyl-to-Alkyne Electron Donation Effects in up to 10-nm-Long, Unimolecular Oligo(p-phenylene ethynyls) (OPEs)” *Organic Materials* **2021**, *3*, 337-345.
15. van der Wetering, C.; Mauel, A.; Sharafi, M.; Aboushousha, R.; Qian, X.; Erickson, C.; MacPherson, M.; Chan, G.; Adcock, I.; Kermai, N. Z.; Schleich, F.; Louis, R.; Bohrsen, E.; D’Alessandro, A.; Wouters, E. F. M.; Reynaert, N. L.; **Li, J.**; Anathy, V.; Wolf, R.; Henderson, C.; Bates, J.; Poynter M. E.; Dixon, A. E.; Irvin, C. G.; van der Vliet, A.; van der Velden, J. L.; Janssen-Heininger, Y. “Glutathione-S-transferase P Promotes Glycolysis in Asthma in Association with Oxidation of Pyruvate Kinase M2” *Redox. Biol.* **2021**, *47*, 102160.
16. Remington, J. M.; Liao, C.; Sharafi, M.; Ste. Marie, E.; Ferrell, J. B.; Hondal, R.; Wargo M. J.; Schneebeli, S. T.; **Li, J.**\* “On the Aggregation State of Synergistic Antimicrobial Peptides” *J. Phys. Chem. Letter* **2020**, *11*, 9501.
17. Remington, J. M.; Ferrell, J. B.; Zorman, M.; Petrucci, A.; Schneebeli, S. T.; **Li, J.**\* “Machine Learning in a Molecular Modeling Course for Chemistry, Biochemistry, and Biophysics Students” *Biophysicist* **2020**, *1*, 11.
18. Rajappan, S. C.; McCarthy, D.; Campbell, J.; Ferrell, J. B.; Sharafi, M.; **Li, J.**\*; Schneebeli, S. T. “Selective Monofunctionalization Enabled by Communicating Reactive Ends in Catalytic Rotaxanes” *Angew. Chem. Int. Ed.* **2020**, *59*, 16668-16674.
19. Sharafi, M.; McKay, K. T.; Ivancic, M.; McCarthy, D. R.; Dudkina, N.; Murphy, K. E.; Rajappan, S. C.; Campbell, J.; Shen, Y.; Badireddy, A. R.; **Li, J.**\*; Schneebeli, S. T. “Size-Selective Catalytic Polymer Acylation with a Molecular Tetrahedron” *Chem* **2020**, *6*, 1469. (*Editor’s Pick in 2020*)
20. Schauer, N. J.; Liu, X.; Magin, R.; Doherty, L.; Chan, W. C.; Ficarro, S. B.; Hu, W.; Roberts, R. M.; Jacob, R. E.; Stolte, B.; Giacomelli, A. O.; Perera, S.; McKay, K.; Boswell, S. A.; Weisberg, E. L.; Chauhan, D.; Dhe-Paganon, S.; Anderson, K. C.; Griffin, J. D.; **Li, J.**; Hahn, W. C.; Sorger, P. K.; Engen, J. R.; Stegmaier, K.; Marto, J. A.; Buhrlage, S. J. “Selective USP7 Inhibition Elicits Cancer Cell Killing through a p53-Dependent Mechanism” *Sci. Rep.* **2020**, *10*, 5324.
21. Zhao, X.; Liao, C.; Ferrell, J. B.; Ma, Y.; Schneebeli, S. T.; **Li, J.**\* “A Top-Down Multiscale Approach to Simulate Peptide Assembly from Monomers” *J. Chem. Theory Comput.* **2019**, *15*, 1514–1522. (*March 2019 Cover*)
22. Ferrell, J. B.; Campbell, J. P.; McCarthy, D. R.; McKay, K.; Hensinger, M.; Srinivasan, R.; Zhao, X.; Wurthmann, A.; **Li, J.**\*; Schneebeli, S. T. “Chemical Exploration with Virtual Reality in Organic Teaching Laboratories” *J. Chem. Educ.* **2019**, *96*, 1961–1966. (*Supplementary Cover*)
23. Liao, C.; Poujol de Molliens, M.; Schneebeli, S. T.; Brewer, M.; Song, G.; Chatenet, D.; Braas, K. M.; May, V.; **Li, J.**\* “Targeting the PAC1 Receptor for Neurological and Metabolic Disorders” *Curr. Top. Med. Chem.* **2019**, *19*, 1399–1417. (*Invited Review*)
24. Chidchob, P.; Offenbartl-Stiegert, D.; McCarthy, D.; **Li, J.**\*; Howorka, S.; Sleiman, H. F. “Spatial Presentation of Cholesterol Units on a DNA Cube as a Determinant of Membrane Protein-Mimicking Functions” *J. Am. Chem. Soc.* **2019**, *141*, 1100–1108.

25. Trinh, T.; Saliba, D.; Liao, C.; Rochambeau, D.; Prinzen, A. L.; **Li, J.**; Sleiman, H. F. “ ‘Printing’ DNA Strand Patterns on Small Molecules with Control of Valency, Directionality and Sequence” *Angew. Chem. Int. Ed.* **2019**, *58*, 3042–3049. (*Special Issue: Women in Chemistry*)
26. Campbell, J. P.; Jaynes, T. J.; Rajappan, S. C.; Sharafi, M.; Ma, Y.; **Li, J.**; Schneebeli, S. T. “Enantioselective Electrophilic Aromatic Nitration: A Chiral Auxiliary Approach” *Angew. Chem. Int. Ed.* **2019**, *58*, 1035–1052. (*Inside Back Cover*)
27. Hameed, U.; Liao, C.; Radhakrishnan, A.; Huser, F.; Aljedani, S.; Zhao, X.; Momin, A.; Melo, F.; Guo, X.; Brooks, C.; Li, Y.; Cui, X.; Gao, X.; Ladbury, J. E.; Jaremko, L.; **Li, J.\***; Arold, S. T. “H-NS Uses an Autoinhibitory Conformational Switch for Environment-Controlled Gene Silencing” *Nucleic Acids Res.* **2019**, *47*, 2666–2680.
28. Liao, C.; May, V.; **Li, J.\*** “PAC1 Receptors: Shapeshifters in Motion” *J. Mol. Neurosci.* **2019**, *68*, 331–339.
29. Trinh, T.; Liao, C.; Toader, V.; Barlog, M.; Bazzi, H.; **Li, J.**; Sleiman, H. F. “DNA-Imprinted Polymer Nanoparticles with Monodispersity and Prescribed DNA-Strand Patterns”, *Nat. Chem.*, **2018**, *10*, 184–192.
30. Heppner, D. E.; Hristova, M.; Ida, T.; Mijuskovic, A.; Dustin, C.; Bogdandi, V.; Fukuto, J. M.; Dick, T. P.; Nagy, P.; **Li, J.**; Akaike, T.; van der Vliet, A. “Cysteine Perthiosulfenic Acid (Cys-SSOH): A Novel Intermediate in Thiol-Based Redox Signaling?” *Redox Biol.* **2018**, *14*, 379–385.
31. Heppner, D. E.; Dustin, C.; Liao, C.; Hristova, M.; Veith, C.; Little, A. A.; Ahlers, B.; White, S. L.; Deng, B.; Lam, Y.; **Li, J.\***; van der Vliet, A. “Direct Cysteine Sulfenylation Drives Activation of the Src Kinase” *Nat. Comm.* **2018**, *9*, 4522.
32. Chan, S.; McCarthy, D.; **Li, J.**; Palczewski, K.; Yuan, S. “Designing Safer Analgesics via  $\mu$ -Opioid Receptor Pathways”, *Trends in Pharma. Sci.*, **2017**, *38*, 1016–1037.
33. Shelley, M.; Selvan, M. E.; Zhao, J.; Babin, V.; Liao, C.; **Li, J.**; Shelley, J. “A New Mixed All-Atom/Coarse-Grained Model for Peptides: Application to Melittin Aggregation in Aqueous Solution” *J. Chem. Theory Comput.* **2017**, *13*, 3881–3897.
34. Liao, C.; Zhao, X.; May, V.; Brewer M.; **Li, J.\*** “Conformational Transitions of the Pituitary Adenylate Cyclase-Activating Polypeptide Receptor, a Human Class B GPCR” *Sci. Rep.* **2017**, *7*, 5427.
35. Sharafi, M.; Campbell, J. P.; Rajappan, S. C.; Dudkina, N.; Gray, D.; Woods, T.; **Li, J.**; Schneebeli, S. T. “Crystal-Packing-Driven Enrichment of Atropoisomers” *Angew. Chem. Int. Ed.* **2017**, *56*, 7203–7207.
36. Murphy, K.; Bocanegra, J.; Liu, X.; Chau, K.; Lee, P.; **Li, J.**; Schneebeli, S. T. “Precise Through Space Control of an Abiotic Electrophilic Aromatic Substitution Reaction” *Nat. Comm.* **2017**, *8*, 14840.
37. Liao, C.; Zhao, X.; Schneebeli, S. T.; Shelley, J.; **Li, J.\*** “Capturing the Multiscale Dynamics of Membrane Protein Complexes with All-Atom, Mixed-Resolution, and Coarse-Grained Models” *Phys. Chem. Chem. Phys.* **2017**, *19*, 9181–9188.

38. Liu, J.; Tian, Z.; Zhou, N.; Liu, X.; Liao, C.; Lei, B.; **Li, J.\***; Zhang, S.; Chen, H. “Targeting the Apoptotic Mcl-1-PUMA Interface with a Dual-acting Compound” *Oncotarget*, **2017**, *8*, 54236–54242.
39. Liao, C.; Zhang, Z.; Kale, J.; Andrews, D. W.; Lin, J.; **Li, J.\*** “Conformational Heterogeneity of Bax Helix 9 Dimer for Apoptotic Pore Formation” *Sci. Rep.* **2016**, *6*, 29502.
40. Sharafi, M.; Weinert, Z.; Liao, C.; **Li, J.\***; Schneebeli, S. T. “Controlled Self-Assembly inside C-Shaped Polyaromatic Strips” *Synlett* **2016**, *27*, 2145–2149.
41. Zhang, Z.; Subramaniam, S.; Kale, J.; Liao, C.; Huang, B.; Brahmabhatt, H.; Condon, S. G. F.; Lapolla, S. M.; Hays, F. A.; Ding, J.; He, F.; Zhang, X. C.; **Li, J.**; Senes, A.; Andrews, D. W.; Lin, J. “BH3-in-Groove Dimerization Initiates and Helix 9 Dimerization Expands Bax Pore Assembly in Membranes” *EMBO J.* **2016**, *35*, 208–236.
42. Liu, X.; Weinert, Z.; Sharafi, M.; Liao, C.; **Li, J.\***; Schneebeli, S. T. “Regulating Molecular Recognition with C-Shaped Strips Attained by Chirality-Assisted Synthesis” *Angew. Chem. Int. Ed.* **2015**, *54*, 12772–12776. (*Inside Cover*)
43. Liao, C.; Selvan, M. E.; Zhao, J.; Slimovitch, J. L.; Schneebeli, S. T.; Shelley, M.; Shelley, J.; **Li, J.\*** “Melittin Aggregation in Aqueous Solutions: Insight from Molecular Dynamics Simulations” *J. Phys. Chem. B*, **2015**, *119*, 10390–10398.

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#### PRE- AND POSTDOCTORAL RESEARCH PUBLICATIONS

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44. Madsen, J.; Sinitskiy, A. V.; **Li, J.**; Voth, G. A. “Highly Coarse-Grained Representations of Transmembrane Proteins” *J. Chem. Theory Comput.* **2017**, *13*, 935–944.
45. **Li, J.**; Ziemba, B.; Falke, J. J.; Voth, G. A. “Interactions of Protein Kinase C- $\alpha$  C1A and C1B Domains with Membranes: A Combined Computational and Experimental Study” *J. Am. Chem. Soc.* **2014**, *136*, 11757–11766.
46. Ziemba, B.; **Li, J.**; Landgraf, K. E.; Knight, J. D.; Voth, G. A.; Falke, J. J. “Single-Molecule Studies Reveal a Hidden Key Step in the Activation Mechanism of Membrane-Bound Protein Kinase C- $\alpha$ ” *Biochemistry*, **2014**, *53*, 1697–1713.
47. Bruns, C. J.; **Li, J.**; Frasconi, M.; Schneebeli, S. T.; Iehl, J.; Jacquot de Rouville, H.; Stupp, S.; Voth, G. A.; Stoddart, J. F. “An Electrochemically and Thermally Switchable Donor-Acceptor [C2]-Daisy Chain Rotaxane” *Angew. Chem. Int. Ed.* **2014**, *53*, 1953–1958.
48. **Li, J.**; Jonsson, A. L.; Beuming, T.; Shelley, J. C.; Voth, G. A. “Ligand-Dependent Activation and Deactivation of the Human Adenosine A2A Receptor” *J. Am. Chem. Soc.* **2013**, *135*, 8749–8759.
49. **Li, J.**; Schneebeli, S. T.; Bylund, J.; Farid, R.; Friesner, R. A. “IDSite: An Accurate Approach to Predict P450-Mediated Drug Metabolism” *J. Chem. Theory Comput.* **2011**, *7*, 3829–3845.
50. Zhao, S. W.; Zhu, K.; **Li, J.**; Friesner, R. A. “Progress in Super Long Loop Prediction” *Proteins* **2011**, *79*, 2920–2935.
51. **Li, J.**; Abel, R.; Zhu, K.; Cao, Y.; Zhao, S. W.; Friesner, R. A. “VSGB 2.0: A Next Generation Energy Model for High Resolution Protein Structural Modeling” *Proteins* **2011**, *79*, 2794–2812.

52. Bochevarov, A.; **Li, J.**; Song, W.; Friesner, R. A.; Lippard, S. J. “Insights into the Different Dioxygen Activation Pathways of Methane and Toluene Monooxygenase Hydroxylases” *J. Am. Chem. Soc.* **2011**, *133*, 7384–7397.
53. Shen, K.; Fu, Y.; **Li, J.**; Liu, L.; Guo, Q. “What Are the p*K*<sub>a</sub> Values of C-H Bonds in Aromatic Heterocyclic Compounds in DMSO?” *Tetrahedron* **2007**, *63*, 1568–1576.
54. **Li, J.**; Fu, Y.; Liu, L.; Guo, Q. “First-Principle Predictions of Basicity of Organic Amines and Phosphines in Acetonitrile” *Tetrahedron* **2006**, *62*, 11801–11813.
55. **Li, J.**; Liu, L.; Fu, Y.; Guo, Q. “What Are the p*K*<sub>a</sub> Values of Organophosphorus Compounds?” *Tetrahedron* **2006**, *62*, 4453–4462.
56. Fu, Y.; Liu, L.; Wang, Y.; **Li, J.**; Yu, T. Q.; Guo, Q. “Quantum-Chemical Predictions of Redox Potentials of Organic Anions in Dimethyl Sulfoxide and Reevaluation of Bond Dissociation Enthalpies Measured by the Electrochemical Methods” *J. Phys. Chem. A* **2006**, *110*, 5874–5886.

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### BOOK CHAPTERS

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1. Liao, C.; May, V.; Li, J. “Chapter 1. Assessment of Conformational State Transitions of Class B GPCRs using Molecular Dynamics”. In “*G Protein-Coupled Receptor Signaling: Methods and Protocols*”; Tiberi M. Eds.; Springer-Nature, **2019**, Page 3–19 ([link](#))

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### PATENTS

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1. May, V.; Brewer, M.; **Li, J.** “Small Molecule Antagonists to PACAP Receptor and Uses Thereof” U.S. Patent Application No.: 62/804,874, **2020**.
2. Schneebeli, S. T.; **Li, J.**; Sharafi, M. “Molecular Tetrahedron Nanocage, Its Preparation, and Uses Thereof”, Patent Application No.: 63/033,764, **2021**.
3. May, V.; Brewer, M.; **Li, J.** “Small molecule antagonist to PACAP receptors: Development of therapeutic compounds for stress-related disorders and chronic pain”, Provisional Patent Application, **2021**.

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### GRANT SUPPORT

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1. “CAREER: Data-Driven Systematic Hierarchical Modeling” (NSF CTMC CHE-1945394). March 2020 – February 2025. Role: PI.
2. “*Structure, Mechanism, and Regulation of PACAP/VIP GPCR Subtypes*” NIH R01GM129431, September 2018 – August 2023. Role: PI.
3. “*S-Glutathionylation Chemistry in Fibrotic Lung Remodeling*” NIH R35HL135828. January 2017 – December 2023. Role: Co-I.
4. “*MRI: Acquisition of a Massive Database to Accelerate Data Science Discovery*” NSF-DMR 2117345, September 2021 – August 2023. Role: co-PI (No Salary Support)

*Three Pending Grant Applications to NIH and NSF.*

## SELECTED AWARDS

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1. NSF CAREER Award, 2020.
2. OpenEye Junior Faculty Award of ACS COMP Division, 2019.
3. Burroughs Wellcome Fund Collaborative Research Award, 2019.
4. Publons Global Peer Review Award of Chemistry, 2018.
5. Biophysical Society CPOW Award, 2018.
6. ACS PRF Doctoral New Investigator Award, 2017.
7. Top 10 Reviewer of *Physical Chemistry Chemical Physics*, 2016.
8. Nomination for the Pew Scholarship, 2016
9. Outstanding Young Researcher Award, Computational Biophysics to Systems Biology Workshop, 2013.
10. ACS Travel Award for the 241<sup>st</sup> ACS National Meeting, Division of Biological Chemistry, 2011.
11. Distinguished Bachelor Dissertation, University of Science and Technology of China, 2006.
12. Guanghua Scholarship, University of Science and Technology of China, 2004.
13. Outstanding Freshwoman Fellowship, University of Science and Technology of China, 2002.

## PROFESSIONAL AFFILIATIONS & ACTIVITIES

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1. Members of the *American Chemical Society*, and the *Biophysical Society*.
2. Peer Reviewer of over 40 journals.
3. Ad hoc Reviewer/Panel Member for NIH (*DDNS*, *MSFD* and *INBRE*), NSF (*DMR* and *CHE*), and ACS (*Petroleum Research Fund*), USIAS Fellowship.
4. Member of the 2017 National Committee (eighth round) on the proposal evaluation for the ANTON2 supercomputer.

## CURRENT GROUP MEMBERS

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Nick Hamilton (Graduate Researcher)

Jonathon Ferrell (Graduate Researcher, CBSB18 Outstanding Young Researcher Awardee)

Subhadra Thapa (Graduate Researcher)

Mica Schenkelberg (Graduate Researcher)

Finley Clark (Undergraduate Researcher, Chemistry Summer Research Fellow/Summer APLE Awardee)

Noah Beckage (Undergraduate Researcher)

## FORMER GROUP MEMBERS

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Former Postdoctoral Researchers:

Dr. Chenyi Liao (Senior Researcher at Dalian Institute of Chemical Physics, CAS, China)

Dr. Yong-Tao Ma (Assistant Professor at Shandong University, China)

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Dr. Jacob Remington (Senior Scientist in Computational Chemistry at Evotec)

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Dr. Kyle McKay (Scientist at Johnson & Johnson, PA)

Dr. Dillon McCarthy (Postdoctoral Fellow at Johnson & Johnson, PA)

Former Undergraduate Researchers:

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Marlo Zorman (Graduate Student in Molecular Engineering at the University of Washington, Seattle)

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