LILLIAN T. CHONG

University of Pittsburgh
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APPOINTMENTS

University of Pittsburgh **Pittsburgh, PA**
Associate Professor (with Tenure) 2012-present
Assistant Professor of Chemistry 2006-2011
Secondary Appointment in Computational & Systems Biology 2006-present
Affiliated Faculty, Joint CMU-Pitt Computational Biology Program 2006-present
Affiliated Faculty, Joint CMU-Pitt Molecular Biophysics/Structural Biology Program 2006-present

EDUCATION

Stanford University/IBM Almaden Research Center **Stanford, CA and San Jose, CA**
Postdoctoral research fellow (Mentors: Vijay Pande/William Swope) 2005-2006

Stanford University **Stanford, CA**
Postdoctoral research fellow (Mentor: Vijay Pande) 2002-2005

University of California at San Francisco (UCSF) **San Francisco, CA**
Ph.D. in Biophysics (Mentors: Peter Kollman/Irwin Kuntz) 1997-2002
Dissertation: *Computational studies of antibody and enzyme catalysis*

Massachusetts Institute of Technology (MIT) **Cambridge, MA**
B.S. in Chemistry 1993-1997
Undergraduate research fellow (Mentor: Bruce Tidor) 1995-1997

AWARDS

U. Pittsburgh Arts & Sciences Bellet Teaching Excellence Award 2017
National Science Foundation CAREER Award 2009-2015
Carnegie Science Emerging Female Scientist Award 2012
Hewlett-Packard Outstanding Junior Faculty Award 2008
Frank M. Goyan Graduate Research Award in Physical Chemistry at UCSF 2002
Burroughs Wellcome Graduate Research Fellowship 2001-2002
National Science Foundation Graduate Research Fellowship 1998-2001
American Institute of Chemists Award 1997
MIT Department of Chemistry Undergraduate Research Award 1997

TEACHING

Graduate course in quantum mechanics (2006-2008); undergraduate courses in quantum mechanics (2009, 2011, 2013, 2016-2019), statistical thermodynamics (2014, 2015, 2017-2020), computational drug discovery (2008-2012, 2014); summer workshop in creative science writing (2017-2019)

SERVICE

Co-organizer of TSRC Workshop on Designing Biomolecular Switches, 2014, 2017
Associate Editor for BMC Biophysics, 2011-2014
National Science Foundation XSEDE Allocations Resource Committee, 2011-2014

INVITED TALKS

(54) OpenEye CUP XX, Santa Fe, 2020.
(53) Biophysical Society Meeting, San Diego, CA, 2020.
(52) Dept. of Biophysics and Physiology, Case Western University, Cleveland, OH, 2019.
(51) MolSSI Software Interoperability Workshop, Brooklyn, NY, 2019.
(50) Free Energy Calculations: Entering the 4th Decade of Adventure, Santa Fe, NM, 2019.
(49) ACS Symposium: Sampling Biomolecules, Orlando, FL, 2019.
(48) Biophysics Program, University of Notre Dame, South Bend, IN, 2019.
(47) Biophysics Program, University of Maryland, College Park, MD, 2018.
(46) National Autonomous University of Mexico, Mexico City, Mexico, 2018.
(45) GRC in Computational Chemistry, West Dover, VT, 2018.
(44) Keynote for Chemical Biophysics Symposium, U. Toronto, Toronto, Canada, 2018.
(43) OpenEye CUP XVII, Santa Fe, NM, 2018
(42) ACS Symposium: Modeling & Measuring Protein-Ligand Kinetics, Washington, DC, 2017
(41) Applied Math and Computational Science Program, U. Pennsylvania, Philadelphia, PA, 2016
(40) ACS Symposium: Multiscale Chemistry, San Diego, CA, 2016
(39) ACS Symposium: Long Time Kinetics of Molecular Events, San Diego, CA, 2016
(38) SFB Polymer Physics, Martin-Luther University Halle-Wittenberg, Halle, Germany, 2016
(37) CECAM Workshop: Free Energy Landscapes for Protein Folding, Zurich, Switzerland, 2015
(36) Plenary Speaker, RosettaCon, Leavenworth, WA, 2015
(35) TSRC Workshop: Chemistry and Dynamics in Complex Environments, Telluride, CO, 2015
(34) Dept. of Biophysics, Johns Hopkins University, Baltimore, MD, 2015
(33) 25th Faltertage Protein Folding Conference, Regensburg, Germany, 2014
(32) ACS Symposium: Tracing Pathways in Biomolecular Simulation, Dallas, TX, 2014
(31) Technical University of Munich, Munich, Germany, 2013
(30) TSRC Workshop: Chemistry and Dynamics in Complex Environments, Telluride, CO, 2013.
(29) Dept. of Chemistry & Biochemistry, UC Santa Barbara, CA, 2013.
(28) UPMC, Sorbonne Universite, Paris, France, 2012.
(27) ACS Workshop: Modeling of Biomolecular Systems at Multi-Resolution, Philadelphia, PA, 2012
(26) TSRC Workshop: Accelerating Reaction Discovery, Telluride, CO, 2012
(25) Midwest Theory Chemistry Conference, Madison, Wisconsin, 2012
(24) Dept. of Chemistry & Biochemistry, U. Missouri, St. Louis, MO, 2012
(23) Young Investigator Lecture, 17th Conversation, SUNY, Albany, NY, 2011
(22) Center for Biotechnology, RPI, Troy, NY, 2011.
(21) Center for Theoretical Biological Physics, UC San Diego, CA, 2011.
(20) SUNY, Stony Brook, NY, 2011.
(19) Rutgers, The State University of New Jersey, New Brunswick, NJ, 2011.
(18) Dept. of Chemistry, Georgia State University, Atlanta, GA, 2011.
(17) Dept. of Chemistry & Biochemistry, Georgia Tech., Atlanta, GA, 2011.
(16) Structural Biology and Biophysics Program, Duke University, Durham, NC, 2011.
(15) Dept. of Chemistry, Temple University, Philadelphia, PA, 2011.
(14) Medicinal Chemistry Program, University of Michigan, Ann Arbor, MI, 2011.
(13) Dept. of Chemistry, University of California, Davis, CA, 2011.
(12) Graduate Program in Biophysics, UC San Francisco, CA, 2011.
(11) Biophysics Program, MIT, Cambridge, MA, 2010.
(10) Dept. of Biochemistry & Molecular Pharmacology, UM Medical School, Worcester, MA, 2010.
(9) Dept. of Chemistry, Boston University, MA, 2010.
(8) TSRC Workshop: Characterizing Energy Landscapes, Telluride, CO, 2010.
(7) Dept. of Chemistry, Ohio State University, Columbus, OH, 2009
(6) Dept. of Chemistry & Biochemistry, University of California, Santa Barbara, CA, 2009.

INVITED TALKS (cont'd)

(5) Dept. of Chemistry, Indiana University of Pennsylvania, Indiana, PA, 2009.
(4) Keynote for MERCURY Conference on Computational Chemistry, Clinton, NY, 2008.
(3) Dept. of Biochemistry, University of Iowa, Iowa City, IA, 2008.
(2) Academy of Sciences of the Czech Republic, Prague, Czech Republic, 2007.
(1) TSRC Workshop: Energy Landscapes, Telluride, CO, 2007.

LILLIAN T. CHONG

PUBLICATIONS ‡Undergraduate researcher

(34) AT Bogetti, B Mostofian, A Dickson, AJ Pratt, AS Saglam, PO Harrison‡, JL Adelman, M Dudek‡, PA Torrillo‡, AJ DeGrave‡, U Adhikari, MC Zwier, DM Zuckerman, and LT Chong. "A suite of tutorials for the WESTPA rare-events sampling software." *Living Journal of Computational Molecular Science*, 1: 10607 (2019).

(33) AS Saglam and LT Chong. "Protein-protein binding pathways and calculations of rate constants using fully-continuous, explicit-solvent simulations." *Chemical Sciences*, 10: 2360 (2019).

(32) AJ DeGrave‡, J-H Ha, SN Loh, and LT Chong. "Large enhancement of response times of a protein conformational switch by computational design." *Nature Comm.*, 9: 1013 (2018).

(31) KT Debiec, MJ Whitley, LMI Koharudin, LT Chong*, and AM Gronenborn*. "Integrating NMR, SAXS, and atomistic simulations: Structure and dynamics of a two-domain protein." *Biophys. J.*, 114: 839-855 (2018). *co-corresponding authors

(30) LT Chong*, AS Saglam, and DM Zuckerman*. "Path-sampling strategies for simulating rare events in biomolecular systems." *Curr. Opin. Struct. Biol.*, 43: 88-94 (2017). *co-corresponding authors

(29) DM Zuckerman* and LT Chong*. "Weighted ensemble simulation: Review of methodology, applications and software." *Ann. Rev. Biophys.*, 46: 43-57 (2017). *co-corresponding authors

(28) AS Saglam, DW Wang‡, MC Zwier, and LT Chong. "Flexibility vs preorganization: Direct comparison of binding kinetics for a disordered peptide and its exact preorganized analogues." *J. Phys. Chem. B*, 121: 10046-10054 (2017).

(27) DS Cerutti, KT Debiec, DA Case, and LT Chong. "Links between the charge model and bonded parameter force constants in biomolecular force fields." *J. Chem. Phys.*, 147: 161730 (2017).

(26) KT Debiec, DS Cerutti, LR Baker‡, AM Gronenborn, DA Case, and LT Chong. "Further along the road less traveled: AMBER ff15ipq, an original protein force field built on a self-consistent physical model." *J. Chem. Theory Comput.*, 12: 3926-3947 (2016).

(25) MC Zwier, AJ Pratt, JL Adelman, JW Kaus‡, DM Zuckerman, and LT Chong. "Efficient atomistic simulation of pathways and calculation of rate constants for a protein-peptide binding process: Application to the MDM2 protein and an intrinsically disordered p53 peptide." *J. Phys. Chem. Lett.*, 7: 3440-3445 (2016).

(24) AS Saglam and LT Chong. "Highly efficient computation of the basal k_{on} using direct simulation of protein-protein association with flexible molecular models." *J. Phys. Chem. B*, 120: 117-122 (2016).

(23) E Suarez, AJ Pratt, LT Chong, and DM Zuckerman. "Estimating first passage time distributions from weighted ensemble simulations and non-Markovian analyses." *Protein Sci.*, 25: 67-78 (2016).

(22) MC Zwier, JL Adelman, JW Kaus‡, AJ Pratt, KF Wong, NB Rego‡, E Suarez, S Lettieri, DW Wang‡, M Grabe, DM Zuckerman, and LT Chong. "WESTPA: An interoperable, highly scalable software package for weighted ensemble simulation and analysis". *J. Chem. Theory Comput.* 11: 800-809 (2015).

PUBLICATIONS (continued)

(21) KT Debiec, AM Gronenborn, and LT Chong. "Evaluating the strength of salt bridges – a comparison of current biomolecular force fields." *J. Phys. Chem. B*, 118: 6561-6569 (2014).

(20) E Suarez, S Lettieri, MC Zwier, CA Stringer, SR Subramanian, LT Chong, and DM Zuckerman. "Simultaneous computation of dynamical and equilibrium information using a weighted ensemble of trajectories." *J. Chem. Theory Comput.*, 10: 2658-2667 (2014).

(19) KM Oshaben, R Salari, DM Caslin, LT Chong, and WS Horne. "The native GCN4 leucine-zipper domain does not uniquely specify a dimeric oligomerization state." *Biochemistry*, 51: 9581-9591 (2012).

(18) R Salari and LT Chong. "Effects of high temperature on desolvation costs of salt bridges across protein binding interfaces: Similarities and differences between implicit and explicit solvent models." *J. Phys. Chem. B,* 116: 2561-2567 (2012).

(17) MT Panteva‡, R Salari, M Bhattacharjee‡, and LT Chong. "Direct observations of shifts in the β-sheet register of a protein-peptide complex using explicit solvent simulations." *Biophys. J.,* 100: L50-L52 (2011).

(16) K Xiong, MC Zwier, NS Myshakina, VM Burger, SA Asher, and LT Chong. "Direct observations of conformational distributions of intrinsically disordered p53 peptides using UV Raman and explicit solvent simulations." *J. Phys. Chem. A*, 115: 9520-9527 (2011).

(15) BM Mills‡ and LT Chong. "Molecular simulations of mutually exclusive folding in a two-domain protein switch." *Biophys. J.*, 100: 756-764 (2011).

(14) MC Zwier, JW Kaus‡, and LT Chong. "Efficient explicit-solvent molecular dynamics simulations of molecular associations: Methane/methane, Na+/Cl-, methane/benzene, and K+/18-crown-6 ether." *J. Chem. Theory Comput.*, 7: 1189-1197 (2011).

(13) JL Adelman, A Scarbrough, MC Zwier, D Bhatt, LT Chong, DM Zuckerman, and M Grabe. "Simulations of the alternating access mechanism of the sodium symporter Mhp1." *Biophys. J.*, 101: 2399-2407 (2011).

(12) MC Zwier and LT Chong. "Reaching biological timescales with all-atom molecular dynamics simulations." *Curr. Opin. Pharmacol.*, 10: 745-752 (2010).

(11) R Salari and LT Chong. "Desolvation costs of salt bridges across protein binding interfaces: Similarities and differences between implicit and explicit solvent models." *J. Phys. Chem. Lett.*, 1: 2844-2848 (2010).

(10) TA Cutler, BM Mills‡, DJ Lubin, LT Chong, and SN Loh. "Effect of interdomain linker length on an antagonistic folding-unfolding equilibrium between two protein domains." *J. Mol. Biol.*, 386: 854-868 (2009).

(9) LT Chong, JW Pitera, WC Swope, and VS Pande. "Comparison of computational approaches for predicting the effects of missense mutations on p53 function." *J. Mol. Graph. Model.,* 27: 978-982 (2009).

Before 2006

(8) LT Chong, WC Swope, JW Pitera, and VS Pande. "Kinetic computational alanine scanning: application to p53 oligomerization." *J. Mol. Biol.*, 357: 1039-1049 (2006).

(7) LT Chong, CD Snow, YM Rhee, and VS Pande. "Dimerization of the p53 oligomerization domain: identification of a folding nucleus by molecular dynamics simulations." *J. Mol. Biol.*, 345: 869-78 (2005).

(6) LT Chong, P Bandyopadhyay, TS Scanlan, ID Kuntz, and PA Kollman. "Direct hydroxide attack is a plausible mechanism for amidase antibody 43C9." *J. Comp. Chem.*, 24: 1371-77 (2003).

(5) TS Lee*, LT Chong*, JD Chodera, and PA Kollman. "An alternative explanation for the catalytic proficiency of orotidine 5'-phosphate decarboxylase." *J. Am. Chem. Soc.*, 123: 12837-48 (2001). *equal authorship

(4) PA Kollman, I Massova, C Reyes, B Kuhn, S Huo, LT Chong, MR Lee, TS Lee, Y Duan, W Wang, O Donini, P Cieplak, J Srinivasan, D Case, and TE Cheatham 3rd. "Calculating structures and free energies of complex molecules: combining molecular mechanics and continuum models." *Accounts of Chemical Research* 33:889-97 (2000).

(3) LT Chong, Y Duan, L Wang, I Massova, PA Kollman. "Molecular dynamics simulation and free energy calculations applied to affinity maturation in antibody 48G7." *Proc. Natl. Acad. Sci. USA* 96: 14330-5 (1999).

(2) K Lin, HS Ateeq, SH Hsiung, LT Chong, CN Zimmerman, A Castro, WC Lee, CE Hammond, S Kalkunte, LL Chen, RB Pepinsky RB, DR Leone, AG Sprague, WM Abraham, A Gill, RR Lobb, and SP Adams. "Selective, tight-binding inhibitors of integrin alpha-4-beta-1 that inhibit allergic airway responses." *J. Med. Chem.*, 42: 920-34 (1999).

(1) LT Chong, SE Dempster, ZS Hendsch, L-P Lee, and B Tidor. "Computation of electrostatic complements to proteins: a case of charge stabilized binding." *Protein Sci.* 7: 206-10 (1998).