LILLIAN T. CHONG

University of Pittsburgh
Department of Chemistry (412) 624-6026
219 Parkman Avenue ltchong@pitt.edu
Pittsburgh, PA 15260 www.pitt.edu/~ltchong

APPOINTMENTS

University of Pittsburgh **Pittsburgh, PA**

Professor of Chemistry	2022-present
Associate Professor (with Tenure)	2012-2021
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

Gordon Bell Special Prize for HPC-based COVID-19 Research	2020
Psivant Discovery Open Science Fellowship	2020, 2021, 2023
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

TEACHING

Graduate course in quantum mechanics (2006-2008); undergraduate courses in quantum mechanics (2009, 2011, 2013, 2016-2022), statistical thermodynamics (2014, 2015, 2017-2020) and computational drug discovery (2008-2012, 2014).

SERVICE

OpenEye, Cadence Scientific Advisory Board (2021-present)
Open Force Field Initiative Advisory Board (2020-present)
Co-organizer of Virtual MolSSI School on Open-Source Software for Rare-Event Sampling Strategies (2021; 145 participants)
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

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PUBLICATIONS

(‡ Indicates undergraduate author)

Perspectives and Reviews

AT Bogetti, MF Presti, SN Loh, and **LT Chong**. Perspective Article: "The next frontier for designing switchable proteins: Rational enhancement of kinetics." *J. Phys. Chem. B*, in press (2021).

- Selected as Journal Cover

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

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

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

Research Articles

AT Bogetti, JMG Leung, JD Russo, S Zhang, JP Thompson, AS Saglam, D Ray, B Mostofian, AJ Pratt, RC Abraham‡, PO Harrison‡, M Dudek‡, PA Torrillo‡, AJ DeGrave‡, U Adhikari, JR Faeder, I Andricioaei, JL Adelman, MC Zwier, DN LeBard, DM Zuckerman, and **LT Chong**. "A suite of tutorials for the WESTPA 2.0 rare-event sampling software [Article v2.0]." *Living J. Comp. Mol. Sci.*, 5: 1655 (2023).

A Dommer, L Casalino, F Kearns, …, DM Zuckerman*, A Mulholland*, T Miller*, S Jha*, A Ramanathan*, **LT Chong***, and RE Amaro*. "#COVIDisAirborne: AI-enabled multiscale computational microscopy of delta SARS-CoV-2 in a respiratory aerosol." *Int. J. High. Perform. C.*, 37: 28-44 (2023).

- Finalist for the 2021 Gordon Bell Special Prize for HPC-based COVID-19 Research.

S Zhang, JP Thompson, J Xia, AT Bogetti, F York, AG Skillman, **LT Chong***, and DN LeBard.* "Mechanistic insights into passive membrane permeability of drug-like molecules from a weighted ensemble of trajectories." *J. Chem. Inf. Model.*, 62: 1891-1904 (2022).

DT Yang, AM Gronenborn*, and **LT Chong***. "Development and validation of fluorinated, aromatic amino acid parameters for use with the AMBER ff15ipq protein force field." *J. Phys. Chem. A*, 126: 2286-2297 (2022).

JD Russo, S Zhang, JMG Leung, AT Bogetti, JP Thompson, A DeGrave, PA Torrillo‡, AJ Pratt, KF Wong, J Xia, J Copperman, JL Adelman, MC Zwier, DN LeBard, DM Zuckerman, and **LT Chong**. "WESTPA 2.0: High-performance upgrades for weighted ensemble simulations and analysis of longer-timescale applications." *J. Chem. Theory Comput.*, 18: 638-649 (2022).

- 2022 Pitt Chemistry David Pratt Award to AT Bogetti and PA Torrillo

T Sztain, SH Ahn, A Bogetti, L Casalino, JA Goldsmith, E Seitz, RS McCool, FL Kearns, F Acosta-Reyes, S Maji, G Mashayekhi, JA McCammon, A Ourmazd, J Frank, JS McLellan, **LT Chong***, and RE Amaro*. "A glycan gate controls opening of the SARS-CoV-2 spike protein." *Nature Chem.*, *Nat. Chem.*, 13: 963-968 (2021).

L Casalino, A Dommer, Z Gaieb, EP Barros, T Sztain, SH Ahn, A Trifan, A Brace, A Bogetti, H Ma, H Lee, M Turilli, S Khalid**, LT Chong**, C Simmerling, DJ Hardy, JDC Maia, JC Phillips, T Kurth, A Stern, L Huang, J McCalpin, M Tatineni, T Gibbs, JE Stone, S Jha, A Ramanathan, and RE Amaro. "AI-driven multiscale simulations illuminate mechanisms of SARS-CoV-2 spike dynamics." *Int. J. High. Perform. C.*, 1-20 (2021).

- Awarded the 2020 Gordon Bell Special Prize for HPC-based COVID-19 Research

AJ DeGrave‡, AT Bogetti, and **LT Chong**. "The RED scheme: Rate-constant estimation from pre-steady state weighted ensemble simulations." *J. Chem. Phys.*, 154: 114111 (2021).

- Selected as Featured and Journal Cover.

PA Torrillo‡, AT Bogetti, and **LT Chong**. "A minimal, adaptive binning scheme for weighted ensemble simulations." *J. Phys. Chem.* A, 125: 1642 (2021).

AT Bogetti, HE Piston‡, JMG Leung, CC Cabalteja, DT Yang, AJ DeGrave, KT Debiec, DS Cerutti, DA Case, WS Horne, and **LT Chong**, L. T. "A twist in the road less traveled: The AMBER ff15ipq-m force field for protein mimetics." *J. Chem. Phys.*, 153: 6, 064101 (2020).

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-event sampling software." *Living J. Comp. Mol. Sci.*, 1: 10607 (2019).

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).
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).

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

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).

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).

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).

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).

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).

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).

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).

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).

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).

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).

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).

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).

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).

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

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).

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).

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).

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).

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).

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

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).

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).

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

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).

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).

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).

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).