**Christopher T. Lee, Ph.D.**

Mechanical and Aerospace Engineering Dept.
University of California, San Diego
9500 Gilman Dr. #0085
SME Bldg. Rm 344A
La Jolla, CA 92093-0085

Email: ctlee@ucsd.edu
Phone: +1 (858) 534-4429
Web Page: ctlee.github.io
Google Scholar: oMawRCAAAAAJ
Orcid: 0000-0002-0670-2308

: @ctlee
in: @ctleeresearch

## EMPLOYMENT

**Hartwell Foundation Postdoctoral Research Fellow**
University of California, San Diego
June 1, 2019 – Current | San Diego, CA

Advisors: Padmini Rangamani & Michael Holst

- Developing a multiscale modeling framework to animate the interactions of systems of molecules in virtual synapses featuring physiologically-derived geometries.

## EDUCATION

**Ph.D. Chemistry**
University of California, San Diego
2013 – 2019 | San Diego, CA

Advisors: Rommie E. Amaro & J. Andrew McCammon

Dissertation: C. T.-K. Lee. "Forging Pathways to Enable Multiscale Modeling of Cellular Scale Phenomena". PhD Dissertation. La Jolla, CA: University of California San Diego, May 2019

- Predictions of passive membrane permeability using physical properties estimated from molecular dynamics simulations.
- Developed biological mesh generation tool `GAMer` and simplicial complex data structure `CASC` to convert structural images into finite elements compatible mesh geometries.

**Computational Physiology Summer Course**
Simula Research Laboratory/Universitetet i Oslo/UCSD
Summer 2017 | Oslo, Norway

- Investigated the affects of drugs on ion channels and the subsequent impact on cellular action potentials using mathematical modeling.

**M.Sc. Chemistry with a Concentration in Biochemistry**
University of Virginia
2011 – 2013 | Charlottesville, VA

Advisors: Linda Columbus & Cameron Mura

Thesis: C. T.-K. Lee. "Broad Specificity of a Zinc-dependent Small Alcohol Dehydrogenase from Thermotoga Maritima Involved in the Glycerol Dismutation Pathway". MSc Thesis. Charlottesville, VA: University of Virginia, May 2012. DOI: 10.18130/V3FD40

**B.Sc. Chemistry & B.A. Computer Science**
University of Virginia
2007 – 2011 | Charlottesville, VA

Advisor: Michael Shirts

- Created the initial prototype of Intermol : a molecular simulation structure, topology, and parameter conversion software.

**High School**
Thomas Jefferson High School for Science and Technology
2003 – 2007 | Alexandria, VA

## HONORS, AWARDS & FELLOWSHIPS

**Fellowships:**

| | | |
|---|---|---|
| 2019 | Hartwell Foundation Postdoctoral Fellowship | The Hartwell Foundation |
| 2018 | Distinguished Graduate Fellowship | UCSD Chem/Biochem |
| 2017-18 | San Diego Diversity Fellowship | UCSD |
| 2017 | Simula Computational Physiology Scholarship | Simula |
| 2014-16 | Molecular Biophysics Training Program, Fellow | UCSD |
| 2011 | NBCR Summer Institute Travel Award | NBCR |

**Honors:**

| | | |
|---|---|---|
| 2019 | Schmidt Science Fellows Finalist | Schmidt Futures |
| 2017 | Scholarship for Scientific Excellence | American Chemical Society CINF |
| 2017 | Biophysical Society Travel Award | Biophysical Society |
| 2017 | Bruno Zimm Award | UCSD Chem/Biochem |
| 2017 | Carol & George Lattimer Award | UCSD Division of Physical Sciences |
| 2015 | Best Poster | UCSD MBTG Annual Retreat |
| Spring 2014 | Teaching Assistant Excellence Award | UCSD Chem/Biochem |
| 2012 | UCSD SHORE Award | UCSD |
| 2011 | Mead Scholar | UVA, Comp. Bio. |

## PUBLICATIONS

† denotes equal contribution, # denotes corresponding author. (h-index = 5, citations = 226 as of 5/13/19)

**Submitted and In Preparation**

[-] **C. T. Lee**†, J. G. Laughlin†, N. Angliviel de La Beaumelle, R. E. Amaro, J. A. McCammon, R. Ramamoorthi, M. J. Holst, and P. Rangamani#. "GAMer 2: A System for 3D Mesh Processing of Cellular Electron Micrographs" (2019). BioRxiv: 10.1101/534479. *Submitted*.

**Peer-Reviewed**

[1] **C. T. Lee**†#, J. B. Moody†, R. E. Amaro, J. A. Mccammon, and M. J. Holst. "The Implementation of the Colored Abstract Simplicial Complex and Its Application to Mesh Generation". en. *ACM Transactions on Mathematical Software* 45.3 (Aug. 2019), pp. 1–20. ISSN: 00983500. DOI: 10.1145/3321515. arXiv: 1807.01417 [cs.MS].

[2] B. C. Taylor, **C. T. Lee**, and R. E. Amaro#. "Structural Basis for Ligand Modulation of the CCR2 Conformational Landscape". *Proc. Natl. Acad. Sci.* 116.17 (Apr. 2019), pp. 8131–8136. ISSN: 0027-8424. DOI: 10.1073/pnas.1814131116. BioRxiv: 10.1101/392068.

[3] B. R. Jagger, **C. T. Lee**, and R. E. Amaro#. "Quantitative Ranking of β-cyclodextrin Ligand Binding Kinetics With SEEKR, a Hybrid MD/BD/Milestoning Approach". *J. Phys. Chem. Lett.* 9.17 (Sept. 2018), pp. 4941–4948. ISSN: 1948-7185. DOI: 10.1021/acs.jpclett.8b02047. ChemRxiv: 10.26434/chemrxiv.6726977.v1. ***Featured on Journal Cover**.

[4] **C. T. Lee** and R. E. Amaro#. "Exascale Computing: A New Dawn for Computational Biology". *Comput. Sci. Eng.* 20.5 (Sept. 2018), pp. 18–25. ISSN: 1521-9615. DOI: 10.1109/MCSE.2018.05329812. ***Special issue on the National Strategic Computing Initiative**.

[5] **C. T. Lee**, J. Comer#, C. Herndon, N. Leung, A. Pavlova, R. V. Swift, C. Tung, C. N. Rowley, R. E. Amaro#, C. Chipot#, Y. Wang#, and J. C. Gumbart#. "Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds". *J. Chem. Inf. Model.* 56.4 (Apr. 2016), pp. 721–733. ISSN: 1549-9596. DOI: 10.1021/acs.jcim.6b00022.

[6] L. W. Votapka†, **C. T. Lee**†, and R. E. Amaro#. "Two Relations to Estimate Membrane Permeability Using Milestoning". *J. Phys. Chem. B* 120.33 (Aug. 2016), pp. 8606–8616. ISSN: 1520-6106. DOI: 10.1021/acs.jpcb.6b02814. ***Special issue J. Andrew McCammon Feschrift**.

[7] J. R. Wagner†, **C. T. Lee**†, J. D. Durrant, R. D. Malmstrom, V. A. Feher, and R. E. Amaro#. "Emerging Computational Methods for the Rational Discovery of Allosteric Drugs". *Chem. Rev.* 116.11 (June 2016), pp. 6370–6390. ISSN: 0009-2665. DOI: 10.1021/acs.chemrev.5b00631.

[8] C. Gray†, C. W. Price†, **C. T. Lee**, A. H. Dewald, M. A. Cline, C. E. McAnany, L. Columbus#, and C. Mura#. "Known structure, unknown function: An inquiry-based undergraduate biochemistry laboratory course". *Biochem. Mol. Biol. Educ.* 43.4 (July 2015), pp. 245–262. ISSN: 14708175. DOI: 10.1002/bmb.20873.

[9] R. D. Malmstrom, **C. T. Lee**, A. T. Van Wart, and R. E. Amaro[#]. "Application of Molecular-Dynamics Based Markov State Models to Functional Proteins". *J. Chem. Theory Comput.* 10.7 (July 2014), pp. 2648–2657. ISSN: 1549-9618. DOI: 10.1021/ct5002363. ***Special issue on free energy**.

## GRANTS AND FUNDING

**TruffleSnout**
**NSF I-Corps** **PI:** C.T. Lee (Co-PI with B. Taylor) FY2017
**Award Amount:** $1000

Team selected to participate in the UCSD NSF I-Corps Winter 2017 cohort. Investigating the potential to commercialize microbiota to assist in growing difficult specialty crops such as truffles.

**Investigating the Structure, Function, and Dynamics of Complex Biological Systems**
**NSF CHE-060063** **PI:** Rommie E. Amaro FY2016
**Award Amount:** PSC Bridges: 1,348,335 SUs, SDSC Comet: 4,881,881 SUs, TACC Stampede: 2,119,112 SUs, SDSC Gordon: 2,860,924 SUs (∼$568,772)

I organized, coordinated collaborations, and wrote this proposal.

**Structural and Dynamical Determinants of Influenza Pathogenicity and Virulence**
**NSF ACI-1440087** **PI:** Rommie E. Amaro 9/1/2014 – 8/31/2015
**Award Amount:** $10,500, 6 million node-hours on Blue Waters (∼$2,400,000)

I contributed to the writing and development of this NSF Petascale Computing Resource Allocation (PRAC) proposal.

**Investigating the Structure, Function, and Dynamics of Complex Biological Systems**
**NSF CHE-060063** **PI:** Rommie E. Amaro FY2015
**Award Amount:** SDSC Gordon: 2,916,406 SUs, TACC Stampede: 4,637,760 SUs (∼$407,770.84)

I contributed to and facilitated the submission of this proposal.

## PRESENTATIONS

### Invited Seminars

[1] "Broad specificity of a zinc-dependent small alcohol dehydrogenase from *Thermotoga maritima* involved in a glycerol dismutation pathway". *University of Virginia*. Charlottesville, VA, Apr. 2011.

### Contributed Talks

[2] "GAMer 2: A system for enabling physical simulations with realistic geometries from cellular electron microscopy". *UCSD MBTG Annual Retreat*. La Jolla, CA, Apr. 2019.

[3] "Investigating Transport Properties With Multi-Scale Computable Mesh Models from Heterogeneous Structural Datasets". *UCSD Industry Interaction Day*. La Jolla, CA, May 2017.

[4] "Investigating Transport Properties With Multi-Scale Computable Mesh Models from Heterogeneous Structural Datasets". *UCSD MBTG Annual Retreat*. La Jolla, CA, May 2017.

[5] "Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds". *UC-wide Symposium for Chemical Sciences*. Lake Arrowhead, CA, Mar. 2016.

[6] "Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds". *UCSD MBTG Seminar*. La Jolla, CA, Jan. 2016.

[7] "Estimating the Local Diffusivity Tensor in Harmonically Constrained Simulations". *UCSD MBTG Seminar*. La Jolla, CA, Mar. 2015.

### Conference Abstracts (Poster)

[8] J. G. Laughlin[†], **C. T. Lee**[†], J. A. McCammon, R. E. Amaro, M. J. Holst, and P. Rangamani. "Modeling the Impact of Spine Apparatus on Signaling and Regulation in Realistic Dendritic Spine Geometries". *Biophysical Society National Meeting*. Baltimore MD, Mar. 2019.

[9] **C. T. Lee**, J. A. McCammon, and R. E. Amaro. "Bridging the Gaps From Molecular to Whole Cell Simulations". *BASF CARA Spring Review*. La Jolla, CA, Mar. 2019.

[10] **C. T. Lee**, J. B. Moody, R. E. Amaro, J. A. McCammon, and M. J. Holst. "GAMer 2.0 Software Toolkit for Adaptive Mesh Generation From Structural Biological Datasets". *Biological Diffusion and Brownian Dynamics Brainstorm 4*. Heidelberg, Germany, Apr. 2018.

[11] **C. T. Lee**, J. B. Moody, R. E. Amaro, J. A. McCammon, and M. J. Holst. "GAMer 2.0 Software Toolkit for Adaptive Mesh Generation From Structural Biological Datasets". *Biophysical Society National Meeting*. San Francisco, CA, Feb. 2018.

[12] **C. T. Lee**, J. B. Moody, R. E. Amaro, J. A. McCammon, and M. J. Holst. "Investigating Transport Properties With Multi-Scale Computable Mesh Models from Heterogeneous Structural Datasets". *American Chemical Society National Meeting*. San Francisco, CA, Apr. 2017. ***Selected for ACS CINF Scholarship for Scientific Excellence**.

[13] **C. T. Lee**, J. B. Moody, R. E. Amaro, J. A. McCammon, and M. J. Holst. "Investigating Transport Properties With Multi-Scale Computable Mesh Models from Heterogeneous Structural Datasets". *Biophysical Society National Meeting*. New Orleans, LA, Feb. 2017. ***Travel Award**.

[14] **C. T. Lee**, L. W. Votapka, J. D. Durrant, J. A. McCammon, and R. E. Amaro. "Correlating Influenza A Polymorphism with Virulence Using an Electrostatic Model". *UCSD MBTG Annual Retreat*. La Jolla, CA, Jan. 2015. ***Best Poster**.

[15] **C. T. Lee**, E. Chen, S. D. Field, M. Kang, J. Allen, H. Bleir, C. W. Price, C. Mura, and L. Columbus. "Purification and characterization of a zinc-dependent glycerol dehydrogenase TM0423 from *Thermotoga maritima*". *ACS Virginia Section*. Charlottesville, VA, Apr. 2011.

[16] **C. T. Lee**, C. W. Price, M. R. Shirts, C. Mura, and L. Columbus. "Known Structure, Unknown Function: Surveying the Ligands of Functionally Uncharacterized Proteins Using a High-Throughput *In Silico* Pipeline". *National Biomedical Computation Resource, Summer Institute*. La Jolla, CA, Aug. 2011.

## PROFESSIONAL SERVICE

**Peer Review:**

- Journal of Chemical Information and Modeling
- Physical Review Journals

**Community Outreach:**

**PNAS Journal Club Panelist**

2018-19

Worked with PNAS Front Matter group to select exciting and recent articles for their science writers to highlight. http://frontmatter.pnas.org/

**BioChemCoRe : Program Director**
University of California, San Diego

Summer 2018

Organized and ran the annual Amaro Lab outreach program. Developed a new 7 week curriculum to teach 9 high school and undergraduate students the basics of computational drug discovery. The students worked to predict the IC50s of a set of Hsp90 inhibitors based upon a provided training set. Tutorials and course material can be found online at https://ctlee.github.io/BioChemCoRe-2018/.

**Student Invited Speaker Committee**
University of California, San Diego

2017

Inaugural member of the UCSD Chemistry & Biochemistry department student invited speaker committee. Helped select and host various speakers. Helped incorporate this organization into the purview of the Chemistry Graduate Student Council to ensure future oversight, funding, and support.

**PRIME Mentor**
University of California, San Diego

2015-17

Promoting Retention Innovation and Mentorship Enrichment program designed to improve graduate student success, completion efforts, develop a culture of effective mentorship, and to further promote a positive environment of inclusivity and diversity.

**BioChemCoRe : Research Mentor**
University of California, San Diego

Summers 2014-17

Instructor and research advisor for this 8 week intensive summer program designed to increase the retention of under-privileged high school students in science.

**Graduate Recruitment Committee**
University of California, San Diego

March 2014-16

Represented the Theoretical and Computational Chemistry Track at incoming graduate student recruitment events. Also contacted interested students to answer questions and inspire interest in joining the department.

**BioLED : Biochemistry Lab Education Resource**
University of Virginia

2011

Developed several modules to teach computational bioinformatic methods which have been successfully incorporated into this one year biochemistry laboratory curriculum. This curriculum is inquiry based. Students investigate a protein that has a determined structure, but the function has not been experimentally investigated.

## TEACHING AND MENTORING

**Teaching Activities:**

- NBCR Data to Structural Models (UCSD, Summer 2016-18)
- BioChemCoRe (UCSD, Summer 2014-18)
- TA, CHEM 167: Medicinal Chemistry (UCSD, Spring 2014)
- TA, CHEM 6bh: General Chemistry II Honors (UCSD, Winter 2014)
- TA, CHEM 6a: General Chemistry I (UCSD, Fall 2013)
- TA, CHEM 4421: Biological Chemistry Lab II (UVA, Spring 2012)
- TA, CHEM 4411: Biological Chemistry Lab I (UVA, Fall 2011)

**Students Supervised:**

Undergraduate Research:

- Chirag Krishna (Bioinformatics, UCSD) 2014-15
- Shelby Friends (Undeclared, Palomar College) NSF REU, Summer 2015
- Aranza S. M. Lopez ENLACE, Summer 2019
- Andrea S. Jacinto ENLACE, Summer 2019

High School Research:

- Mason Holst (Canyon Crest Academy) 2018-2019
- Gray Thoron (San Diego Metropolitan Regional and Technical) 2018

BioChemCoRe (Summers of various years, UG and HS):
Hillary Pratt, Aditya Ravipathi, Kevin Cheng, Michael Murphy, Divya Ghoshal, Cynthia Chen, Jessie Gan, Gaurie Gunasekaran, Tyler Kraft, Dhruv Kumar, Emmanuel Ledesma, Kien Malarney, Neel Mittal, Michael Tu