

# Christopher T. Lee, Ph.D.

San Diego Supercomputer Center, E-290  
9500 Gilman Drive #0347  
La Jolla CA 92093-0347

Email: [ctlee@ucsd.edu](mailto:ctlee@ucsd.edu)  
Phone: +1 (858) 822-5285  
Web Page: [ctleelab](http://ctleelab)  
Google Scholar: [oMawRCAAAAAAJ](https://scholar.google.com/citations?user=oMawRCAAAAAAJ)  
Orcid: [0000-0002-0670-2308](https://orcid.org/0000-0002-0670-2308)

: [@ctlee](https://twitter.com/ctlee)  
: [@ctlee](https://github.com/ctlee)  
: [@ctleelab](https://in.linkedin.com/in/ctleelab)

## EMPLOYMENT

---

### Assistant Professor

Dept. Molecular Biology, University of California San Diego

 July 1, 2024 – Present

 San Diego, CA

### Kavli Institute of Brain and Mind Postdoctoral Scholar

University of California San Diego

 June 1, 2019 – June 30, 2024

 San Diego, CA

Advisors: Padmini Rangamani [↗](#) & Michael Holst [↗](#)

- Kavli Institute of Brain and Mind Postdoctoral Fellow 2022–2024
- Hartwell Foundation Postdoctoral Fellow 2019–2021
- Developing a multiscale modeling framework to animate the interactions of systems of molecules in virtual synapses featuring physiologically-derived geometries.
- Developed biological mesh generation tool GAMer to convert structural images into finite elements compatible mesh 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 1, 2019 [↗](#)

- Predictions of passive membrane permeability using physical properties estimated from molecular dynamics simulations
- Developed simplicial complex data structure CASC to support robust mesh generation codes for electrostatics calculations
- Applied enhanced sampling techniques to predict protein and ligand binding dynamics

### 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 1, 2012. DOI: [10.18130/V3FD40](https://doi.org/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

## HONORS, AWARDS & FELLOWSHIPS

---

### ►Fellowships:

2022-2023	KIBM Postdoctoral Scholar <a href="#">↗</a> (\$50k/year × 2)	Kavli Institute of Brain and Mind
2019-21	Hartwell Foundation Postdoctoral Fellowship <a href="#">↗</a> (\$100k)	The Hartwell Foundation
2018	Distinguished Graduate Fellowship <a href="#">↗</a>	UCSD Chem/Biochem
2017 – 2018	San Diego Diversity Fellowship	UCSD
2017	Simula Computational Physiology Scholarship	Simula
2014-16	Molecular Biophysics Training Program (NIH T32 GM008326)	UCSD
2011	NBCR Summer Institute Travel Award	NBCR

### ►Honors:

2019	Postdoc. Appreciation Award <a href="#">↗</a>	UCSD OPRSA
2019	Schmidt Science Fellows Finalist <a href="#">↗</a>	Schmidt Futures
2017	Scholarship for Scientific Excellence <a href="#">↗</a>	American Chemical Society CINF
2017	Biophysical Society Travel Award	Biophysical Society
2017	Bruno Zimm Award <a href="#">↗</a>	UCSD Chem/Biochem
2017	Carol & George Lattimer Award <a href="#">↗</a>	UCSD Division of Physical Sciences
2017	NSF Innovation Corps	UCSD
2015	Best Poster	UCSD MBTG Annual Retreat
Sp. 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.

### ►Submitted and In Preparation

- [-] K. Venkatraman, **C. T. Lee**, and I. Budin#. “Setting the curve: the biophysical properties of lipids in mitochondrial form and function” (Aug. 26, 2024). *Submitted*.
- [-] E. A. Francis†, J. Laughlin†, J. S. Dokken, H. Finsberg, **C. T. Lee**, M. E. Rognes#, and P. Rangamani#. “Spatial Modeling Algorithms for Reactions and Transport (SMART) in Biological Cells” (May 25, 2024). *Submitted*. Preprint: [BioRxiv](#) [↗](#).

### ►Peer-Reviewed

- [1] J. M. Griswold, M. Bonilla-Quintana†, R. Pepper†, **C. T. Lee**†, S. Raychaudhuri, S. Ma, Q. Gan, S. Syed, C. Zhu, M. Bell, M. Suga, Y. Yamaguchi, U. V. Nägerl, G. Knott, P. Rangamani#, and S. Watanabe#. “Membrane mechanics dictate axonal morphology and function”. *Nature Neuroscience* (July 1, 2024). *in press*. Preprint: [BioRxiv](#) [↗](#).
- [2] **C. T. Lee**, M. Bell, M. Bonilla-Quintana, and P. Rangamani#. “Biophysical modeling of synaptic plasticity”. *Annual Review of Biophysics* 53.1 (Feb. 21, 2024). DOI: [10.1146/annurev-biophys-072123-124954](https://doi.org/10.1146/annurev-biophys-072123-124954).
- [3] K. Venkatraman, **C. T. Lee**†, G. C. Garcia†, A. Mahapatra†, G. Perkins, K.-Y. Kim, H. A. Pasolli, S. Phan, J. Lippincott-Schwartz, M. Ellisman, P. Rangamani#, and I. Budin#. “Cristae formation is a mechanical buckling event controlled by the inner membrane lipidome”. *The EMBO Journal* 42.24 (Dec. 11, 2023), e114054. DOI: [10.15252/embj.2023114054](https://doi.org/10.15252/embj.2023114054). Preprints: [BioRxiv](#) [↗](#), PMC: [10054968](https://pubmed.ncbi.nlm.nih.gov/10054968/).
- [4] J. G. Laughlin, J. S. Dokken, H. N. T. Finsberg, E. A. Francis, **C. T. Lee**, M. E. Rognes, and P. Rangamani#. “SMART: Spatial Modeling Algorithms for Reaction and Transport”. *Journal of Open Source Software* 8.90 (Oct. 19, 2023), p. 5580. DOI: [10.21105/joss.05580](https://doi.org/10.21105/joss.05580). Preprint: [arXiv: 10.48550/arXiv.2306.07368](https://arxiv.org/abs/10.48550/arXiv.2306.07368) [q-bio].
- [5] H. Nakamura#, E. Rho, **C. T. Lee**, K. Itoh, D. Deng, S. Watanabe, S. Razavi, H. T. Matsubayashi, C. Zhu, E. Jung, P. Rangamani, S. Watanabe, and T. Inoue#. “ActuAtoR, a Listeria-inspired molecular tool for generating force in living cells: Controlled deformation of intracellular organizations”. *Cell Reports* 42.10 (Sept. 20, 2023), p. 113089. DOI: [10.1016/j.celrep.2023.113089](https://doi.org/10.1016/j.celrep.2023.113089). Preprint: PMC: [10872831](https://pubmed.ncbi.nlm.nih.gov/10872831/).
- [6] F. Yuan, **C. T. Lee**, J. Houser, A. Sangani, L. Wang, E. Lafer, P. Rangamani#, and J. Stachowiak. “The ins and outs of membrane bending by intrinsically disordered proteins”. *Science Advances* 9.27 (July 7, 2023), eadg3485. DOI: [10.1126/sciadv.adg3485](https://doi.org/10.1126/sciadv.adg3485). Preprints: [BioRxiv](#) [↗](#), PMC: [10328403](https://pubmed.ncbi.nlm.nih.gov/10328403/).
- [7] M. K. Bell, **C. T. Lee**, and P. Rangamani#. “Spatiotemporal Modelling Reveals Geometric Dependence of AMPAR Dynamics on Dendritic Spine Morphology”. *The Journal of Physiology* 601.15 (Nov. 23, 2022), pp. 3329–3350. DOI: [10.1113/JP283407](https://doi.org/10.1113/JP283407). Preprints: [BioRxiv](#) [↗](#), PMC: [9280073](https://pubmed.ncbi.nlm.nih.gov/9280073/).
- [8] C. Zhu, **C. T. Lee**#, and P. Rangamani#. “Mem3DG: An open-source software framework for 3-D membrane mechanochemical dynamics using discrete differential geometry on triangulated meshes”. *Biophys. Reports* 2.3 (Sept. 14, 2022), p. 100062. DOI: [10.1016/j.bpr.2022.100062](https://doi.org/10.1016/j.bpr.2022.100062). Preprints: [BioRxiv](#) [↗](#), PMC: [9495267](https://pubmed.ncbi.nlm.nih.gov/9495267/).

- [9] I. López-Peña, **C. T. Lee**, J. J. Rivera, M. J. Tauber, and J. E. Kim<sup>#</sup>. “Role of the Triplet State and Protein Dynamics in the Formation and Stability of the Tryptophan Radical in an Apoazurin Mutant”. *J. Phys. Chem. B* 126 (Aug. 17, 2022). DOI: [10.1021/acs.jpcc.2c02441](https://doi.org/10.1021/acs.jpcc.2c02441). Preprint: PMC: [9483921](https://pubmed.ncbi.nlm.nih.gov/3483921/).
- [10] M. K. Bell<sup>†</sup>, M. V. Holst<sup>†</sup>, **C. T. Lee**, and P. Rangamani<sup>#</sup>. “Dendritic Spine Morphology Regulates Calcium-Dependent Synaptic Weight Change”. *J. Gen. Physiol.* 154.8 (July 1, 2022), e202112980. DOI: [10.1085/jgp.202112980](https://doi.org/10.1085/jgp.202112980). Preprints: BioRxiv [↗](https://doi.org/10.1101/2021.07.01.450073), PMC: [9280073](https://pubmed.ncbi.nlm.nih.gov/3280073/).
- [11] J. L. Gan, D. Kumar, C. Chen, B. C. Taylor, B. R. Jagger, R. E. Amaro<sup>#</sup>, and **C. T. Lee**<sup>#</sup>. “Benchmarking Ensemble Docking Methods in D3R Grand Challenge 4”. *J. Comput. Aided. Mol. Des.* 36.2 (Feb. 1, 2022), pp. 87–99. DOI: [10.1007/s10822-021-00433-2](https://doi.org/10.1007/s10822-021-00433-2). Preprints: BioRxiv [↗](https://doi.org/10.1101/2021.02.01.428095), PMC: [8907095](https://pubmed.ncbi.nlm.nih.gov/3907095/).
- [12] R. Mendelsohn<sup>†</sup>, G. C. Garcia<sup>†</sup>, T. M. Bartol, **C. T. Lee**, P. Khandelwal, E. Liu, D. J. Spencer, A. Husar, E. A. Bushong, S. Phan, G. Perkins, M. H. Ellisman, A. Skupin, T. J. Sejnowski<sup>#</sup>, and P. Rangamani<sup>#</sup>. “Morphological Principles of Neuronal Mitochondria”. *J. Comp. Neurol.* 530.6 (Nov. 1, 2021), pp. 886–902. DOI: [10.1002/cne.25254](https://doi.org/10.1002/cne.25254). Preprints: BioRxiv [↗](https://doi.org/10.1101/2021.08.11.454699), PMC: [8831469](https://pubmed.ncbi.nlm.nih.gov/38831469/).
- [13] **C. T. Lee**, M. Akamatsu, and P. Rangamani<sup>#</sup>. “Value of Models for Membrane Budding”. *Curr. Opin. Cell Biol.* 71 (Aug. 1, 2021), pp. 38–45. DOI: [10.1016/j.ceb.2021.01.011](https://doi.org/10.1016/j.ceb.2021.01.011). Preprint: PMC: [8328869](https://pubmed.ncbi.nlm.nih.gov/3328869/).
- [14] T. Hempel, M. J. del Razo<sup>†</sup>, **C. T. Lee**<sup>†</sup>, B. C. Taylor<sup>†</sup>, R. E. Amaro<sup>#</sup>, and F. Noé<sup>#</sup>. “Independent Markov Decomposition: Towards modeling kinetics of biomolecular complexes”. *Proc. Natl. Acad. Sci.* 118.31 (July 28, 2021). DOI: [10.1073/pnas.2105230118](https://doi.org/10.1073/pnas.2105230118). Preprints: BioRxiv [↗](https://doi.org/10.1101/2021.07.28.450663), PMC: [8346863](https://pubmed.ncbi.nlm.nih.gov/38346863/).
- [15] R. Vasani, M. P. Rowan, **C. T. Lee**, G. R. Johnson, P. Rangamani, and M. Holst<sup>#</sup>. “Applications and Challenges of Machine Learning to Enable Realistic Cellular Simulations”. *Front. Phys.* 7 (Jan. 21, 2021). DOI: [10.3389/fphy.2019.00247](https://doi.org/10.3389/fphy.2019.00247). (2019 Frontiers in Physics Editors Choice). Preprint: arXiv: [1911.05218](https://arxiv.org/abs/1911.05218) [[physics.bio-ph](https://arxiv.org/html/1911.05218v1)].
- [16] **C. T. Lee**<sup>†</sup>, J. G. Laughlin<sup>†</sup>, N. Angliviel de La Beaumelle, R. E. Amaro, J. A. McCammon, R. Ramamoorthi, M. J. Holst, and P. Rangamani<sup>#</sup>. “3D Mesh Processing Using GAMer 2 to Enable Reaction-Diffusion Simulations in Realistic Cellular Geometries”. *PLOS Comp. Biol.* 16.4 (Apr. 6, 2020), e1007756. DOI: [10.1371/journal.pcbi.1007756](https://doi.org/10.1371/journal.pcbi.1007756). Preprints: arXiv: [1901.11008](https://arxiv.org/abs/1901.11008) [[q-bio.QM](https://arxiv.org/html/1901.11008v1)], BioRxiv [↗](https://doi.org/10.1101/2019.04.24.256611), PMC: [6716611](https://pubmed.ncbi.nlm.nih.gov/6716611/).
- [17] **C. T. Lee**<sup>#</sup>, J. G. Laughlin, J. B. Moody, R. E. Amaro, J. A. McCammon, M. J. Holst, and P. Rangamani<sup>#</sup>. “An Open Source Mesh Generation Platform for Biophysical Modeling Using Realistic Cellular Geometries”. *Biophys. J.* 118.5 (Mar. 10, 2020), pp. 1003–1008. DOI: [10.1016/j.bpj.2019.11.3400](https://doi.org/10.1016/j.bpj.2019.11.3400). Preprints: arXiv: [1909.04781](https://arxiv.org/abs/1909.04781) [[physics.comp-ph](https://arxiv.org/html/1909.04781v1)], BioRxiv [↗](https://doi.org/10.1101/2019.09.11.296475), PMC: [7063475](https://pubmed.ncbi.nlm.nih.gov/7063475/).
- [18] **C. T. Lee**<sup>†#</sup>, J. B. Moody<sup>†</sup>, R. E. Amaro, J. A. Mccammon, and M. J. Holst. “The Implementation of the Colored Abstract Simplicial Complex and Its Application to Mesh Generation”. *ACM Trans. Math. Softw.* 45.3 (Aug. 8, 2019), pp. 1–20. DOI: [10.1145/3321515](https://doi.org/10.1145/3321515). Preprints: arXiv: [1807.01417](https://arxiv.org/abs/1807.01417) [[cs.MS](https://arxiv.org/html/1807.01417v1)], PMC: [6716611](https://pubmed.ncbi.nlm.nih.gov/6716611/).
- [19] B. C. Taylor, **C. T. Lee**, and R. E. Amaro<sup>#</sup>. “Structural Basis for Ligand Modulation of the CCR2 Conformational Landscape”. *Proc. Natl. Acad. Sci.* 116.17 (Apr. 23, 2019), pp. 8131–8136. DOI: [10.1073/pnas.1814131116](https://doi.org/10.1073/pnas.1814131116). Preprints: BioRxiv [↗](https://doi.org/10.1101/2019.04.11.296475), PMC: [6486717](https://pubmed.ncbi.nlm.nih.gov/6486717/).
- [20] B. R. Jagger, **C. T. Lee**, and R. E. Amaro<sup>#</sup>. “Quantitative Ranking of  $\beta$ -cyclodextrin Ligand Binding Kinetics With SEEKR, a Hybrid MD/BD/Milestoning Approach”. *J. Phys. Chem. Lett.* 9.17 (Sept. 6, 2018), pp. 4941–4948. DOI: [10.1021/acs.jpclett.8b02047](https://doi.org/10.1021/acs.jpclett.8b02047). (Featured on Journal Cover). Preprints: ChemRxiv [↗](https://doi.org/10.26434/chemrxiv-2018-08-01), PMC: [6443090](https://pubmed.ncbi.nlm.nih.gov/6443090/).
- [21] **C. T. Lee** and R. E. Amaro<sup>#</sup>. “Exascale Computing: A New Dawn for Computational Biology”. *Comput. Sci. Eng.* 20 (Aug. 30, 2018), pp. 18–25. DOI: [10.1109/MCSE.2018.05329812](https://doi.org/10.1109/MCSE.2018.05329812). (Special issue on the National Strategic Computing Initiative). Preprint: PMC: [6458592](https://pubmed.ncbi.nlm.nih.gov/6458592/).
- [22] L. W. Votapka<sup>†</sup>, **C. T. Lee**<sup>†</sup>, and R. E. Amaro<sup>#</sup>. “Two Relations to Estimate Membrane Permeability Using Milestoning”. *J. Phys. Chem. B* 120.33 (Aug. 25, 2016), pp. 8606–8616. DOI: [10.1021/acs.jpcc.6b02814](https://doi.org/10.1021/acs.jpcc.6b02814). (Special issue J. Andrew McCammon Festschrift). Preprint: PMC: [5002937](https://pubmed.ncbi.nlm.nih.gov/5002937/).
- [23] J. R. Wagner<sup>†</sup>, **C. T. Lee**<sup>†</sup>, J. D. Durrant, R. D. Malmstrom, V. A. Feher, and R. E. Amaro<sup>#</sup>. “Emerging Computational Methods for the Rational Discovery of Allosteric Drugs”. *Chem. Rev.* 116.11 (June 8, 2016), pp. 6370–6390. DOI: [10.1021/acs.chemrev.5b00631](https://doi.org/10.1021/acs.chemrev.5b00631). Preprint: PMC: [4901368](https://pubmed.ncbi.nlm.nih.gov/4901368/).
- [24] **C. T. Lee**, J. Comer<sup>#</sup>, C. Herndon, N. Leung, A. Pavlova, R. V. Swift, C. Tung, C. N. Rowley, R. E. Amaro<sup>#</sup>, C. Chipot<sup>#</sup>, Y. Wang<sup>#</sup>, and J. C. Gumbart<sup>#</sup>. “Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds”. *J. Chem. Inf. Model.* 56.4 (Apr. 25, 2016), pp. 721–733. DOI: [10.1021/acs.jcim.6b00022](https://doi.org/10.1021/acs.jcim.6b00022). Preprint: PMC: [5280572](https://pubmed.ncbi.nlm.nih.gov/5280572/).
- [25] C. Gray<sup>†</sup>, C. W. Price<sup>†</sup>, **C. T. Lee**, A. H. Dewald, M. A. Cline, C. E. McAnany, L. Columbus<sup>#</sup>, and C. Mura<sup>#</sup>. “Known Structure, Unknown Function: An Inquiry-Based Undergraduate Biochemistry Laboratory Course”. *Biochem. Mol. Biol. Educ.* 43.4 (July 8, 2015), pp. 245–262. DOI: [10.1002/bmb.20873](https://doi.org/10.1002/bmb.20873). Preprint: PMC: [4758391](https://pubmed.ncbi.nlm.nih.gov/4758391/).

- [26] R. D. Malmstrom, C. T. Lee, A. T. Van Wart, and R. E. Amaro<sup>#</sup>. “Application of Molecular-Dynamics Based Markov State Models to Functional Proteins”. *J. Chem. Theory Comput.* 10.7 (July 8, 2014), pp. 2648–2657. DOI: [10.1021/ct5002363](https://doi.org/10.1021/ct5002363). (Special issue on free energy). Preprint: PMC: [4248791](https://pubmed.ncbi.nlm.nih.gov/4248791/).

## ►Book Chapters

- [27] C. T. Lee<sup>#</sup> and P. Rangamani<sup>#</sup>. “Modeling the Mechanochemical Feedback for Membrane-Protein Interactions Using a Continuum Mesh Model”. *Biophysical Approaches for the Study of Membrane Structure—Part B: Theory and Simulations*. Ed. by M. Deserno and T. Baumgart. Vol. 701. Methods in Enzymology. Academic Press, July 16, 2024, pp. 387–424. DOI: [10.1016/bs.mie.2024.03.016](https://doi.org/10.1016/bs.mie.2024.03.016).

## GRANTS AND FUNDING

---

### ►Completed Funding

#### Innovative Research Grant [↗](#)

KIBM

PI: C. T. Lee

📅 7/1/2021 -- 6/30/2022

Award Amount: \$50,000 (\$38,000 to CTL)

- co-PIs: Courtney Glavis-Bloom, Casey Vanderlip, John Reynolds, Sammy Weiser Novak, Uri Manor, Miriam K. Bell, Mayte Bonilla-Quintana, Padmini Rangamani
- Investigating the relationships between synaptic energy efficiency and age-related cognitive decline
- Hosted summer internships for 2 high school aged students

#### TruffleSnout

NSF I-Corps

PI: C. T. Lee and B. C. Taylor

📅 FY2017

Award Amount: \$1000

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

## PRESENTATIONS

---

### ►Invited

- [1] *Telluride Workshop – Complexity in the Chemistry and Physics of Lipid Membranes*. Telluride, CO, June 2025.
- [2] *Dept. of Molecular Biophysics*. La Jolla, CA, Apr. 2024.
- [3] *Telluride Workshop – Complexity in the Chemistry and Physics of Lipid Membranes*. Telluride, CO, June 2023.
- [4] *International Meshing Roundtable*. Amsterdam, Netherlands, Mar. 2023.
- [5] *Simula*. La Jolla, CA, Aug. 2021.
- [6] *Society for Brain Mapping and Therapeutics*. Los Angeles, CA, Mar. 2021.
- [7] *UCSD CSE Pixel Cafe*. La Jolla, CA, Nov. 2020.
- [8] *Center for Computational Mathematics*. La Jolla, CA, May 2019.
- [9] *University of Virginia*. Charlottesville, VA, Apr. 2011.

### ►Contributed Talks

- [10] *UCSD MBTG Annual Retreat*. La Jolla, CA, Apr. 2019.
- [11] *UCSD Industry Interaction Day*. La Jolla, CA, May 2017.
- [12] *UCSD MBTG Annual Retreat*. La Jolla, CA, May 2017.
- [13] *UC-wide Symposium for Chemical Sciences*. Lake Arrowhead, CA, Mar. 2016.
- [14] *UCSD MBTG Seminar*. La Jolla, CA, Jan. 2016.
- [15] *UCSD MBTG Seminar*. La Jolla, CA, Mar. 2015.

### ►Conference Abstracts (Poster)

- [16] *Biophysical Society National Meeting*. Philadelphia, PA, Feb. 2024.
- [17] *Biophysical Society National Meeting*. San Diego, CA, Feb. 2023.
- [18] *Biophysical Society National Meeting*. San Francisco, CA, Apr. 2022.
- [19] *Biophysical Society National Meeting*. San Diego CA, Feb. 2020.
- [20] *BASF CARA Spring Review*. La Jolla, CA, Mar. 2019.
- [21] *Biophysical Society National Meeting*. Baltimore MD, Mar. 2019.
- [22] *Biological Diffusion and Brownian Dynamics Brainstorm 4*. Heidelberg, Germany, Apr. 2018.

- [23] *Biophysical Society National Meeting*. San Francisco, CA, Feb. 2018.
- [24] *American Chemical Society National Meeting*. San Francisco, CA, Apr. 2017. (Selected for ACS CINF Scholarship for Scientific Excellence).
- [25] *Biophysical Society National Meeting*. New Orleans, LA, Feb. 2017. (Travel Award).
- [26] *UCSD MBTG Annual Retreat*. La Jolla, CA, Jan. 2015. (Best Poster).
- [27] *National Biomedical Computation Resource, Summer Institute*. La Jolla, CA, Aug. 2011.
- [28] *ACS Virginia Section*. Charlottesville, VA, Apr. 2011.

## PROFESSIONAL SERVICE

---

### ›Peer Review:

- AFOSR LRIR Review
- Chemistry and Physics of Lipids
- Journal of Chemical Information and Modeling
- Journal of Physical Chemistry
- Physical Review Journals
- Nature Communications Biology
- Soft Matter

### ›Community Outreach:

#### ENLACE Mentor [↗](#)

University of California San Diego

📅 Summer 2019

- Supervised summer research for two undergraduate level students from Mexico
- The students constructed geometric mesh models of neuronal mitochondria from electron tomograms

#### PNAS Journal Club Panelist [↗](#)

fontmatter.pnas.org

📅 2018-19

- Worked with PNAS Front Matter group to select exciting and recent articles for their science writers to highlight

#### BioChemCoRe [↗](#): Program Director

University of California San Diego

📅 Summer 2018

- Organized and ran the annual Amaro Lab outreach program
- Developed a 7 week curriculum to teach computational drug discovery and soft skills (teach science as we do science)
- 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 Chem. & Biochem. student invited speaker committee
- Selected and hosted various speakers on behalf of the students
- Lobbied to add the seminar series into the responsibilities of the Chemistry Graduate Student Council to ensure future oversight, funding, and support

#### PRIME Mentor

University of California San Diego

📅 2015 - 17

- Mentor "Promoting Retention Innovation and Mentorship Enrichment" for incoming graduate students
- 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

- 8 week annual summer outreach program seeking to increase retention of under-privileged and diverse students in science
- Organized and presented teaching materials on computational chemistry methods
- Sponsored and advised student research projects

#### Graduate Recruitment Committee

University of California San Diego

📅 March 2014-16

- Represented the Theoretical and Computational Chemistry Track at incoming graduate recruitment events
- Answered questions from interested students

## BioLED: Biochemistry Lab Education Resource

University of Virginia

📅 2011

- Developed inquiry based modules to teach computational bioinformatics
- Contributed to curriculum where 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

#### ›Mentorship:

##### Graduate Research:

- Xiaoyi Wu (Physics, UCSD) 2023 – Present
- Natalia Reis (Chemistry and Biochemistry, UCSD) 2023
- Cuncheng Zhu (Mechanical Engineering, UCSD) 2019 – 2022
- Justin Laughlin (Mechanical Engineering, UCSD) 2019 – 2022
- Miriam Bell (Mechanical Engineering, UCSD) 2019 – 2022
  - NDSEG Fellow
- Andrew Nguyen (Mechanical Engineering, UCSD) 2020 – 2022
  - Honorable Mention–2020 NSF GRFP

##### Undergraduate Research:

- Andrew Nguyen (Bioengineering, UCSD) 2019 – 2020
- Justin Oshiro (Mechanical Engineering, UCSD) 2019 – 2020
- Meagan P. Rowan (Bioengineering, UCSD) 2019 – 2020
- Andrea S. Jacinto (Chemistry, UNAM) ENLACE, Summer 2019
- Aranza S. M. Lopez (Nanoengineering, UPSIN) ENLACE, Summer 2019
- Nils Angliviell de La Beaumelle (Environmental Engineering, UCSD) 2018 – 2019
- Chirag Krishna (Bioinformatics, UCSD) 2014 – 15
  - Amgen Scholar
- Shelby Friends (Undeclared, Palomar College) NSF REU, Summer 2015

##### High School Research:

- Rishabh Bhutani (Rocklin High School) 2024 – Present
- Nandana Madhukara (Canyon Crest Academy) 2022 – Present
  - 1st Place Computational Systems (Medical)–2023 California Sci. & Eng. Fair [🔗](#)
  - 2nd Place–2023 UCLA Brain Research Award [🔗](#)
  - Invited to International Sci. & Eng. Fair
- Aditi Telang (Olympian High School) 2021 – 2022
- Kavya Gupta (Westview High School) 2020 – 2023
  - Invited to American Junior Academy of Science Conference
- Eleanor Jung (Mt. Carmel High School) 2020 – 2023
  - 4th Place–2021 Intermountain JSHS
  - Grand Award Runner-Up–2021 Greater San Diego Sci. & Eng. Fair
  - 4th Place Comp. Bio. and Bioinform.–2021 International Sci. & Eng. Fair (ISEF) [🔗](#)
- Maven Holst (Canyon Crest Academy) 2018 – 2021
  - 1st Place–2019 Greater San Diego Sci. & Eng. Fair
  - 2nd Place–2019 California Sci. & Eng. Fair
  - Invited to International Sci. & Eng. Fair
- Jessie Gan (San Diego Jewish Academy) 2018 – 2021
  - Finalist (Top 40)–2021 Regeneron Science Talent Search Finalist [🔗](#)
  - 2020 Davidson Fellow [🔗](#)
  - Awards from Sigma Xi and Broadcom MASTERS, California Sci. & Eng. Fair, Greater San Diego Sci. & Eng. Fair
- Dhruv Kumar (Rancho Bernardo High School) 2018 – 2021

- Cynthia Chen (Canyon Crest Academy)
- Gray Thoron (San Diego Metropolitan Regional and Technical)

2018 – 2019  
2018

BioChemCoRe (Summers of years 2014 – 2018, UG and HS):

Hillary Pratt, Aditya Ravipathi, Kevin Cheng, Cynthia Chen, Jessie Gan, Michael Murphy, Divya Ghoshal, Gaurie Gunasekaran, Tyler Kraft, Dhruv Kumar, Emmanuel Ledesma, Kien Malarney, Neel Mittal, Michael Tu

#### PROFESSIONAL MEMBERSHIPS

---

2006 – 2008	AAAS
2016 – 2018	American Chemical Society
2016 –	Biophysical Society
2024 –	ASCB

#### REFERENCES

---

Available upon request