





# David D. L. Minh

Updated 11th March 2024

Robert E. Frey, Jr. Endowed Chair in Chemistry  
Associate Professor, Department of Chemistry  
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## Highlights

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### Research

- Coauthored 55 peer-reviewed journal articles, 35 as corresponding author.
- Cited over 1400 times with an h-index of 22, according to [Google scholar](#).
- Principal investigator of three federal grants and co-investigator of one.

### Teaching

- Mentored 12 Ph.D. students, 5 M.S. students.
- Taught 10 different courses from the freshman to graduate level.

### Academic Service

- Serving as [Associate Director](#) for the Center for Interdisciplinary Scientific Computation.
- [Conducted over 100 manuscript reviews](#).

### Honors

- Appointed as inaugural Robert E. Frey, Jr. Endowed Faculty in Chemistry in 2020.
- Named as one of 40 under 40 Chicago Scientists by Halo Cures in 2019.
- Recipient of the 2019 Sigma Xi Junior Faculty Award, Illinois Tech chapter, in recognition of Outstanding Accomplishments in Research and Scholarship.
- Recipient of a 2018 College of Science Dean's Excellence Award in Research, at the Junior Level.

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# Biographical

## Professional History

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2022 – present	<b>Affiliated Faculty, Department of Biology</b> , Illinois Institute of Technology (Illinois Tech), Chicago, IL
2020 – present	<b>Robert E. Frey, Jr. Endowed Faculty in Chemistry</b> , Illinois Tech, Chicago, IL
2019 – present	<b>Associate Professor</b> (tenured), Department of Chemistry, Illinois Tech
2018 – present	<b>Associate Director</b> , Center for Interdisciplinary Scientific Computation, Illinois Tech
2013 – 2019	<b>Assistant Professor</b> (tenure-track), Department of Chemistry, Illinois Tech
2011 – 2013	<b>Postdoctoral Research Associate</b> , Duke University, Durham, NC
2009 – 2011	<b>Director’s Postdoctoral Fellow</b> , Argonne National Laboratory, Argonne, IL
2007 – 2009	<b>Postdoctoral Trainee</b> , National Institutes of Health, Bethesda, MD

## Education

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2004 – 2007	<b>Ph.D. in Physical Chemistry</b> , University of California, San Diego. Thesis Title: Free Energy Reconstruction from Irreversible Single-Molecule Pulling Experiments. Recipient of Molecular Biophysics Training Grant and Aguoron Kamen and Kaplan Fellowship.
2000 – 2003	<b>B.A. in Chemistry</b> , University of California, Berkeley. Recipient of Chancellor’s Scholarship (Berkeley’s most prestigious scholarship) and National Merit Scholarship.

## Awards

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2020	College of Letters and Science Nominee, Michael J. Graf IIT Teaching and Advising Innovation Award.
2019	40 under 40 Chicago Scientists. Selected by Halo Cures.
2019	Sigma Xi Junior Faculty Award, in recognition of Outstanding Accomplishments in Research and Scholarship. Awarded by the Illinois Tech chapter of the scientific research honor society, Sigma Xi.
2018	College of Science Dean’s Excellence Award in Research, at the Junior Level
2012	OpenMM Visiting Scholar (at Stanford)
2009 – 2011	Director’s Postdoctoral Fellowship
2007 – 2009	Postdoctoral Intramural Research Training Award
2005 – 2007	NIH Molecular Biophysics Training Grant
2004 – 2005	Aguoron Kamen and Kaplan Fellowship
2000 – 2003	UC Berkeley Chancellor’s Scholarship
2000 – 2003	National Merit Scholarship

# Research

## Publications

\* publication in which I am a corresponding author.

† undergraduate coauthor.

## Peer-Reviewed Articles

 <https://orcid.org/0000-0002-4802-2618>

- 1 Nguyen, H. H., Tufts, J., & **Minh, D. D. L.\***. (2024). On Inactivation of the Coronavirus Main Protease. *Journal of Chemical Information and Modeling*, acs.jcim.3c01518. <https://doi.org/10.1021/acs.jcim.3c01518>
- 2 Bobby, M. L., Fearon, D., Ferla, M., Filep, M., Koekemoer, L., Robinson, M. C., The COVID Moonshot Consortium†, Chodera, J. D., Lee, A. A., London, N., Von Delft, A., Von Delft, F., Achdout, H., Aimon, A., Alonzi, D. S., Arbon, R., Aschenbrenner, J. C., Balcomb, B. H., Bar-David, E., Barr, H., Ben-Shmuel, A., Bennett, J., Bilenko, V. A., Borden, B., Boulet, P., Bowman, G. R., Brewitz, L., Brun, J., Bvnbs, S., Calmiano, M., Carbery, A., Carney, D. W., Cattermole, E., Chang, E., Chernyshenko, E., Clyde, A., Coffland, J. E., Cohen, G., Cole, J. C., Contini, A., Cox, L., Croll, T. I., Cvitkovic, M., De Jonghe, S., Dias, A., Donckers, K., Dotson, D. L., Douangamath, A., Duberstein, S., Dudgeon, T., Dunnett, L. E., Eastman, P., Erez, N., Eyermann, C. J., Fairhead, M., Fate, G., Fedorov, O., Fernandes, R. S., Ferrins, L., Foster, R., Foster, H., Fraisse, L., Gabizon, R., García-Sastre, A., Gawriljuk, V. O., Gehrtz, P., Gileadi, C., Giroud, C., Glass, W. G., Glen, R. C., Glinert, I., Godoy, A. S., Gorichko, M., Gorrie-Stone, T., Griffen, E. J., Haneef, A.†, Hassell Hart, S., Heer, J., Henry, M., Hill, M., Horrell, S., Huang, Q. Y. J., Huliak, V. D., Hurley, M. F. D., Israely, T., Jajack, A., Jansen, J., Jnoff, E., Jochmans, D., John, T., Kaminow, B., Kang, L., Kantsadi, A. L., Kenny, P. W., Kiappes, J. L., Kinakh, S. O., Kovar, B., Krojer, T., La, V. N. T., ... Zvornicanin, S. N. (2023). Open science discovery of potent noncovalent SARS-CoV-2 main protease inhibitors. *Science*, 382, eabo7201. <https://doi.org/10.1126/science.abo7201>
- 3 La, V. N. T., & **Minh, D. D. L.\***. (2023). Bayesian Regression Quantifies Uncertainty of Binding Parameters from Isothermal Titration Calorimetry More Accurately Than Error Propagation. *International Journal of Molecular Sciences*, 24, 15074. <https://doi.org/10.3390/ijms242015074>
- 4 La, V. N. T., Nicholson, S.†, Haneef, A.†, Kang, L., & **Minh, D. D. L.\***. (2023). Inclusion of Control Data in Fits to Concentration–Response Curves Improves Estimates of Half-Maximal Concentrations. *Journal of Medicinal Chemistry*, 66, 12751–12761. <https://doi.org/10.1021/acs.jmedchem.3c00107>
- 5 Nicholson, S.†, **Minh, D. D. L.**, & Eisenberg, R. (2023). H-Bonds in Crambin: Coherence in an  $\alpha$ -Helix. *ACS Omega*, 8, 13920–13934. <https://doi.org/10.1021/acsomega.3c00181>
- 6 Willow, S. Y., Kang, L., & **Minh, D. D. L.\***. (2023). Learned Mappings for Targeted Free Energy Perturbation between Peptide Conformations. *Journal of Chemical Physics*, 159, 124104. <https://doi.org/10.1063/5.0164662>

- 7 Nguyen, T. H., La, V. N. T., Burke, K., & **Minh, D. D. L.\***. (2022). Bayesian regression and model selection for isothermal titration calorimetry with enantiomeric mixtures. *PLoS ONE*, *17*, e0273656. <https://doi.org/10.1371/journal.pone.0273656>
- 8 Tuz, K., Yuan, M., Hu, Y., Do, T. T. T., Willow, S. Y., DePaolo-Boisvert, J. A., Fuller, J. R., **Minh, D. D. L.**, & Juárez, O. (2022). Identification of the riboflavin cofactor-binding site in the *Vibrio cholerae* ion-pumping NQR complex: A novel structural motif in redox enzymes. *Journal of Biological Chemistry*, *298*, 102182. <https://doi.org/10.1016/j.jbc.2022.102182>
- 9 Willow, S. Y., Yuan, M., Juárez, O., & **Minh, D. D. L.\***. (2021). Electrostatics and water occlusion regulate covalently-bound flavin mononucleotide cofactors of *Vibrio cholerae* respiratory complex NQR. *Proteins: Structure, Function, and Bioinformatics*, *89*, prot.26158. <https://doi.org/10.1002/prot.26158>
- 10 Menzer, W. M.†, Xie, B., & **Minh, D. D. L.\***. (2020). On Restraints in End-Point Protein-Ligand Binding Free Energy Calculations. *Journal of Computational Chemistry*, *41*, 573–586. <https://doi.org/10.1002/jcc.26119>
- 11 **Minh, D. D. L.\***. (2020). Alchemical Grid Dock (AlGDock): Binding Free Energy Calculations between Flexible Ligands and Rigid Receptors. *Journal of Computational Chemistry*, *41*, 715–730. <https://doi.org/10.1002/jcc.26036>
- 12 Nguyen, T. H., & **Minh, D. D. L.\***. (2020). Implicit ligand theory for relative binding free energies: II. An estimator based on control variates. *Journal of Physics Communications*, *4*, 115010. <https://doi.org/10.1088/2399-6528/abcbac>
- 13 Spiridon, L., Sulea, T. A., **Minh, D. D. L.**, & Petrescu, A. J. (2020). Robosample: Rigid-body molecular simulation based on robot mechanics. *BBA - General Subjects*, *1864*, 129616. <https://doi.org/10.1016/j.bbagen.2020.129616>
- 14 Willow, S. Y., Xie, B., Lawrence, J.†, Eisenberg, R. S., & **Minh, D. D. L.\***. (2020). On the Polarization of Ligands by Proteins. *Physical Chemistry Chemical Physics*, *22*, 12044–12057. <https://doi.org/10.1039/d0cp00376j>
- 15 Xie, B., Yao, Q., Xiang, J., & **Minh, D. D. L.\***. (2020). A Structural Model for Bax $\Delta$ 2-Mediated Activation of Caspase 8-Dependent Apoptosis. *International Journal of Molecular Sciences*, *21*, 5476. <https://doi.org/10.3390/ijms21155476>
- 16 Fang, X., Osipiuk, J., Chakravarthy, S., Yuan, M., Menzer, W.†, Nissen, D., Liang, P., Raba, D. A., Tuz, K., Howard, A. J., Joachimiak, A., **Minh, D. D. L.**, & Juárez, O. (2019). Conserved residue His-257 of *Vibrio cholerae* flavin transferase ApbE plays a critical role in substrate binding and catalysis. *Journal of Biological Chemistry*, *294*, 13800–13810. <https://doi.org/10.1074/jbc.RA119.008261>
- 17 Nguyen, T. H., Ngo, V., Castro Zerba, J.†, Noskov, S. Y., & **Minh, D. D. L.\***. (2019). Nonequilibrium path-ensemble averages for symmetric protocols. *Journal of Chemical Physics*, *151*, 194103. <https://doi.org/10.1063/1.5121306>
- 18 Raba, D. A., Yuan, M., Fang, X., Menzer, W. M.†, Xie, B., Liang, P., Tuz, K., **Minh, D. D. L.**, & Juárez, O. (2019). Role of Subunit D in Ubiquinone-Binding Site of *Vibrio cholerae* NQR: Pocket Flexibility and Inhibitor Resistance. *ACS Omega*, *4*, 19324–19331. <https://doi.org/10.1021/acsomega.9b02707>

- 19 Xie, B., & **Minh, D. D. L.\***. (2019). Alchemical Grid Dock (AlGDock) calculations in the D3R Grand Challenge 3. *Journal of Computer-Aided Molecular Design*, *33*, 61–69. <https://doi.org/10.1007/s10822-018-0143-9>
- 20 Menzer, W.†, Li, C., Sun, W., Xie, B., & **Minh, D. D. L.\***. (2018). Simple Entropy Terms for End-Point Binding Free Energy Calculations. *Journal of Chemical Theory and Computation*, *14*, 6035–6049. <https://doi.org/10.1021/acs.jctc.8b00418>
- 21 **Minh, D. D. L.\***. (2018). Power transformations improve interpolation of grids for molecular mechanics interaction energies. *Journal of Computational Chemistry*, *39*, 1200–1207. <https://doi.org/10.1002/jcc.25180>
- 22 Nguyen, T. H., & **Minh, D. D. L.\***. (2018). Implicit ligand theory for relative binding free energies. *Journal of Chemical Physics*, *148*, 104114. <https://doi.org/10.1063/1.5017136>
- 23 Nguyen, T. H., Rustenburg, A. S., Krimmer, S. G., Zhang, H., Clark, J. D.†, Novick, P. A., Branson, K., Pande, V. S., Chodera, J. D., & **Minh, D. D. L.\***. (2018). Bayesian analysis of isothermal titration calorimetry for binding thermodynamics. *PLoS ONE*, *13*, e0203224. <https://doi.org/10.1371/journal.pone.0203224>
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- 25 Raba, D. A., Rosas-Lemus, M., Menzer, W. M.†, Li, C., Fang, X., Liang, P., Tuz, K., **Minh, D. D. L.**, & Juárez, O. (2018). Characterization of the Pseudomonas aeruginosa NQR Complex, a Bacterial Proton Pump with Roles in Autopoisoning Resistance. *Journal of Biological Chemistry*, *293*, 15664–15677. <https://doi.org/10.1074/jbc.RA118.003194>
- 26 Ren, S., Sun, X., Wang, H., Nguyen, T. H., Sadeghipour, N., Xu, X., Kang, C. S., Liu, Y., Xu, H., Wu, N., Chen, Y., Tichauer, K., **Minh, D. D. L.**, & Chong, H.-S. (2018). Design, Synthesis, and Biological Evaluation of Novel Polyaminocarboxylate Ligand-Based Theranostic Conjugate for Antibody-Targeted Cancer Therapy and Near-Infrared Optical Imaging. *ChemMedChem*, *13*, 2606–2617. <https://doi.org/10.1002/cmdc.201800598>
- 27 Xie, B., Clark, J. D.†, & **Minh, D. D. L.\***. (2018). Efficiency of stratification for ensemble docking using reduced ensembles. *Journal of Chemical Information and Modeling*, *58*, 1915–1925. <https://doi.org/10.1021/acs.jcim.8b00314>
- 28 Onuk, E., Badger, J., Wang, Y. J., Bardhan, J., Chishti, Y., Akcakaya, M., Brooks, D. H., Erdogmus, D., **Minh, D. D. L.**, & Makowski, L. (2017). Effects of Catalytic Action and Ligand Binding on Conformational Ensembles of Adenylate Kinase. *Biochemistry*, *56*, 4559–4567. <https://doi.org/10.1021/acs.biochem.7b00351>
- 29 Spiridon, L., & **Minh, D. D. L.\***. (2017). Hamiltonian Monte Carlo with Constrained Molecular Dynamics as Gibbs Sampling. *Journal of Chemical Theory and Computation*, *13*, 4649–4659. <https://doi.org/10.1021/acs.jctc.7b00570>
- 30 Tuz, K., Li, C., Fang, X., Raba, D. A., Liang, P., **Minh, D. D. L.**, & Juárez, O. (2017). Identification of the Catalytic Ubiquinone-binding Site of Vibrio cholerae Sodium-dependent NADH Dehydrogenase: A NOVEL UBIQUINONE-BINDING MOTIF. *Journal of Biological Chemistry*, *292*, 3039–3048. <https://doi.org/10.1074/jbc.M116.770982>



- 31 Xie, B., Nguyen, T. H., & **Minh, D. D. L.\***. (2017). Absolute Binding Free Energies between T4 Lysozyme and 141 Small Molecules: Calculations Based on Multiple Rigid Receptor Configurations. *Journal of Chemical Theory and Computation*, *13*, 2930–2944. <https://doi.org/10.1021/acs.jctc.6b01183>
- 32 **Minh, D. D. L.**, Minh, D. L., & Nguyen, A. L. (2016). Layer Sampling. *Communications in Statistics - Simulation and Computation*, *45*, 73–100. <https://doi.org/10.1080/03610918.2013.854907>
- 33 Nguyen, T. H., & **Minh, D. D. L.\***. (2016). Intermediate Thermodynamic States Contribute Equally to Free Energy Convergence: A Demonstration with Replica Exchange. *Journal of Chemical Theory and Computation*, *12*, 2154–2161. <https://doi.org/10.1021/acs.jctc.6b00060>
- 34 **Minh, D. D. L.**, & Minh, D. L. (2015). Understanding the Hastings Algorithm. *Communications in Statistics - Simulation and Computation*, *44*, 332–349. <https://doi.org/10.1080/03610918.2013.777455>
- 35 **Minh, D. D. L.**, & Makowski, L. (2013). Wide-angle X-ray solution scattering for protein-ligand binding: Multivariate curve resolution with bayesian confidence intervals. *Biophysical Journal*, *104*, 873–883. <https://doi.org/10.1016/j.bpj.2012.12.019>
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- 37 **Minh, D. D. L.\***. (2012b). Implicit ligand theory: Rigorous binding free energies and thermodynamic expectations from molecular docking. *Journal of Chemical Physics*, *137*, 104106. <https://doi.org/10.1063/1.4751284>
- 38 Minh, D. L., **Minh, D. D. L.**, & Nguyen, A. L. (2012). Regenerative Markov chain Monte Carlo for any distribution. *Communications in Statistics - Simulation and Computation*, *41*, 1745–1760. <https://doi.org/10.1080/03610918.2011.615433>
- 39 Makowski, L., Gore, D. B., Mandava, S., **Minh, D. D. L.**, Park, S., Rodi, D. J., & Fischetti, R. F. (2011). X-ray Solution Scattering Studies of the Structural Diversity Intrinsic to Protein Ensembles. *Biopolymers*, *95*, 531–542. <https://doi.org/10.1002/bip.21631>
- 40 **Minh, D. D. L.\***, & Chodera, J. D. (2011). Estimating equilibrium ensemble averages using multiple time slices from driven nonequilibrium processes: Theory and application to free energies, moments, and thermodynamic length in single-molecule pulling experiments. *Journal of Chemical Physics*, *134*, 024111. <https://doi.org/10.1063/1.3516517>
- 41 **Minh, D. D. L.\***, & Vaikuntanathan, S. (2011). Density-dependent analysis of nonequilibrium paths improves free energy estimates II. A Feynman-Kac formalism. *Journal of Chemical Physics*, *134*, 034117. <https://doi.org/10.1063/1.3541152>
- 42 Nilmeier, J. P., Crooks, G. E., **Minh, D. D. L.**, & Chodera, J. D. (2011). PNAS Plus: Nonequilibrium candidate Monte Carlo is an efficient tool for equilibrium simulation. *Proceedings of the National Academy of Sciences of the United States of America*, *108*, E1009–E1018. <https://doi.org/10.1073/pnas.1106094108>

- 43 **Minh, D. D. L.\***. (2010). Optimized replica gas estimation of absolute integrals and partition functions. *Physical Review E*, 82, 31132. <https://doi.org/10.1103/PhysRevE.82.031132>
- 44 Qin, S. B., **Minh, D. D. L.**, McCammon, J. A., & Zhou, H.-X. X. (2010). Method to Predict Crowding Effects by Postprocessing Molecular Dynamics Trajectories: Application to the Flap Dynamics of HIV-1 Protease. *Journal of Physical Chemistry Letters*, 1, 107–110. <https://doi.org/10.1021/jz900023w>
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- 46 **Minh, D. D. L.**, & Adib, A. B. (2009). Path integral analysis of Jarzynski's equality: Analytical results. *Physical Review E*, 79, 021122. <https://doi.org/10.1103/PhysRevE.79.021122>
- 47 **Minh, D. D. L.\***, & Chodera, J. D. (2009). Optimal estimators and asymptotic variances for nonequilibrium path-ensemble averages. *Journal of Chemical Physics*, 131, 134110. <https://doi.org/10.1063/1.3242285>
- 48 Makowski, L., Rodi, D. J., Mandava, S., **Minh, D. D. L.**, Gore, D. B., & Fischetti, R. F. (2008). Molecular crowding inhibits intramolecular breathing motions in proteins. *Journal of Molecular Biology*, 375, 529–546. <https://doi.org/10.1016/j.jmb.2007.07.075>
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- 51 Amaro, R. E., **Minh, D. D. L.**, Cheng, L. S., Lindstrom William M, J., Olson, A. J., Lin, J.-H. H., Li, W. W., & McCammon, J. A. (2007). Remarkable loop flexibility in avian influenza N1 and its implications for antiviral drug design. *Journal of the American Chemical Society*, 129, 7764–7765. <https://doi.org/10.1021/ja0723535>
- 52 **Minh, D. D. L.\***. (2007). Multidimensional Potentials of Mean Force from Biased Experiments along a Single Coordinate. *Journal of Physical Chemistry B*, 111, 4137–4140. <https://doi.org/10.1021/jp068656n>
- 53 **Minh, D. D. L.\***, Hamelberg, D., & McCammon, J. A. (2007). Accelerated entropy estimates with accelerated dynamics. *Journal of Chemical Physics*, 127, 154105. <https://doi.org/10.1063/1.2794754>
- 54 **Minh, D. D. L.\***. (2006). Free-energy reconstruction from experiments performed under different biasing programs. *Physical Review E*, 74, 61120. <https://doi.org/10.1103/PhysRevE.74.061120>
- 55 **Minh, D. D. L.\***, Chang, C.-e. A., Trylska, J., Tozzini, V., & McCammon, J. A. (2006). The influence of macromolecular crowding on HIV-1 protease internal dynamics. *Journal of the American Chemical Society*, 128, 6006–6007. <https://doi.org/10.1021/ja060483s>



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<https://doi.org/10.1529/biophysj.105.069336>

## Oral Presentations at National and International Conferences

† an invited talk. ‡ financial support from the conference.

- 2023 Learned Mappings for Targeted Free Energy Perturbation between Peptide Conformations. *125th Statistical Mechanics Conference*. New Brunswick, NJ
- Energy-Preserving Auto-Encoding and Decoding of Atomistic Protein Structure. *Gibbs Conference on Biological Thermodynamics* Carbondale, IL. Presented by Joseph DePaolo-Boisvert.
- Energy-Preserving Auto-Encoding and Decoding of Atomistic Protein Structure. *American Chemical Society Fall 2023 National Meeting* San Francisco, CA. Presented by Joseph DePaolo-Boisvert.
- Assessment of density-based clustering for the construction of Markov state models. *American Chemical Society Fall 2023 National Meeting* San Francisco, CA. Presented by Hong Ha Nguyen.
- Binding pose prediction using absolute binding free energy calculations. *Free Energy Methods in Drug Design*. Cambridge, MA. †
- Linear systems analysis of atomic interactions using molecular dynamics: A study of the mu opioid receptor. *American Chemical Society Spring 2023 National Meeting* Indianapolis, IN. Presented by Stanley Nicholson.
- H-bonds in Crambin: Coherence in an alpha-helix. *Asia Pacific Conference of Theoretical and Computational Chemistry*. Quy Nhon, Vietnam. †
- Binding pose prediction using absolute binding free energy calculations. *Free Energy Methods in Drug Design*. Cambridge, MA. †
- 2022 Inclusion of control data in fitting to dose-response curves. *American Chemical Society Fall 2022 National Meeting* Chicago, IL. Presented by Van La.
- Symmetry-breaking mechanisms of the SARS-CoV-2 main protease. *42nd Midwest Enzyme Chemistry Conference* Chicago, IL. Presented by Hong Ha Nguyen.
- Symmetry-breaking mechanisms of the SARS-CoV-2 main protease. *American Chemical Society Fall 2022 National Meeting* Chicago, IL. Presented by Hong Ha Nguyen.
- 2021 Large-scale Free Energy Calculations with Implicit Ligand Theory. *Free Energy Methods in Drug Design*. † (online)
- 2020 Large-scale Free Energy Calculations with Implicit Ligand Theory. *OpenEye CUP XX*. Santa Fe, NM. †‡
- 2019 New Computational Tools for Discovering Drugs and Chemical Probes. *Annual Conference of the Romanian Society of Biochemistry and Molecular Biology*. Iasi, Romania. †‡
- Fast Binding Free Energy Methods. *Free Energy Calculations: Entering the Fourth Decade of Adventure in Chemistry and Biophysics*. Santa Fe, NM. †

## Oral Presentations at National and International Conferences (continued)

- 2018 Insights from molecular simulations of the ion-pumping NADH-ubiquinone oxidoreductase (NQR). *256th American Chemical Society National Meeting*, in “Membrane Protein Simulations & Free Energy Approaches”. Boston, MA. †
- 2017 Hamiltonian Monte Carlo with Constrained Molecular Dynamics as Gibbs Sampling. *Recent Advances in Modeling Rare Events (RARE 2017)*. Agra, India. †‡
1. Enhanced sampling with constrained dynamics 2. Protein-ligand binding free energies using multiple rigid receptor structures. *Free Energy Calculations: Three Decades of Adventure in Chemistry and Biophysics*. Telluride, CO. †
- Protein-Ligand Binding Free Energy Calculations based on Multiple Rigid Receptor Conformations. *Beyond Kds: New computational methods to address challenges in drug discovery*. Lausanne, Switzerland. †‡
- Enhanced sampling of molecular conformations with rigid body dynamics. *From Computational Biophysics to Systems Biology (CBSB 2017)*, Cincinnati, OH.
- 2016 Emerging methods for second-stage virtual screening. *Free Energy Methods in Drug Design*. Boston, MA. †
- 2015 Predicting the Mechanism of Anthocyanin-Induced Insulin Sensitization with Molecular Modeling. *250th American Chemical Society National Meeting*, in “Phytonutrients: Thinking Beyond the ‘Essential’ Nutrient Box”. Boston, MA. †‡
- Absolute Binding Free Energies between Ligands and Rigid Protein Conformations: Precise Estimation and Improved Activity Classification. *Computational Chemical Biology*. Cairns, Australia. †‡
- Developing efficient free energy methods on Open Science Grid. *Open Science Grid All Hands Meeting*. Evanston, IL. †
- 2014 Finding Needles in Haystacks: Enzyme Activity Classification based on Implicit Ligand Theory. *Midwest Enzyme Chemistry Conference*. Evanston, IL.
- From molecular docking to standard binding free energies: clearing the trail marked by implicit ligand theory. *Molecular Recognition*. Telluride, CO. †
- Nonequilibrium Driven Processes for Rare Event Sampling/Traversing Thermodynamic State Space. *Recent Advances in Modeling Rare Events (RARE 2014)*. Kerala, India. †‡
- Implicit Ligand Theory: Protein-Ligand Binding Free Energies for the Masses? *Free Energy Methods in Drug Design*. Boston MA. †
- 2013 Molecular Docking Scores Based on Implicit Ligand Theory, a Rigorous Formalism for Binding Free Energies. *245th American Chemical Society National Meeting*, in Thomas Kuhn Paradigm Shift Award Symposium. New Orleans, LA.
- 2010 Lag and the Convergence of Nonequilibrium Free Energy Estimates. *Free Energy Methods in Drug Design*, Vertex Pharmaceuticals, Boston MA. May 17, 2010. †
- 2009 Two Ways are Better Than One: Optimized Free Energies from Bidirectional Single-Molecule Force Spectroscopy. *Condensed Matter Summer School: Nonequilibrium Statistical Mechanics* Boulder, CO. ‡

## Contributions to Open-Source Software

- Led development of **AlGDock**, an open-source computational chemistry program for performing binding free energy calculations.
- Contributed to development of **bitc**, data analysis software for isothermal titration calorimetry measurements.

## Research Funding

2023 – 2024	Bridging Biochemical and Antiviral Activities of ASAP MPro inhibitors. <i>National Institutes of Health subaward from Sloan-Kettering Institute for Cancer Research</i> . \$212K to IIT. PI.
2021 – 2025	Development of a new class of antibiotics against <i>Vibrio Cholerae</i> Na <sup>+</sup> -NQR. <i>National Institutes of Health</i> . \$2.7M to IIT. Co-I. PI Oscar Juarez.
2019 – 2020	The Redox-Coupled Conformational Mechanism of Na <sup>+</sup> -NQR. <i>National Research Council at the National Academies of Science</i> . MCB190085P. 115,000 Molecular Dynamics Simulation Units on Anton 2, a supercomputer specialized for biomolecular simulation. PI. Co-PI Oscar Juarez.
2019 – 2022	Collaborative Research: CDS&E: Elucidating Binding using Bayesian Inference to Integrate Multiple Data Sources. <i>National Science Foundation</i> . CHE 1905324. \$495K over 3 years. PI. Co-Is John Chodera and Lulu Kang.
2018 – 2022	Entropy for End-Point and FFT-Based Binding Free Energy Calculations. <i>National Institutes of Health</i> 1 R01 GM127712-01. \$1.33M over 4 years. PI. Co-I Oscar Juarez.
2015 – 2018	Sound-stage Virtual Screening Based on Implicit Ligand Theory. <i>National Institutes of Health</i> 1 R15 GM114781-01. \$337K over 3 years. PI.
2014	Elucidating the Mechanism of Anthocyanin-Induced Insulin Sensitization. <i>IIT Educational and Research Initiative Fund</i> . \$25K for 1 year. Co-PI with Britt Burton-Freeman and Indika Edirisinghe.

## Teaching

### Trainee Awards

2023	Kilpatrick Scholarship, for the best undergraduate student in chemistry. To undergraduate student David Cooper.
2023	Undergraduate Karl Menger Award, for the best undergraduate student in applied mathematics. To coterminal student Stanley Nicholson.
2023	Fellowship from the NSF Graduate Research Fellowship Program. To coterminal student Stanley Nicholson.
2022	Kilpatrick Lecture Symposium, Second Prize. To graduate student James Tufts.
2022	Illinois Tech Welcome Week Student Research Event, Outstanding Graduate Research Award in the College of Computing. To coterminal student Stanley Nicholson.
2021	Illinois Tech Biology/Chemistry/Food Science and Nutrition/Physics Poster Day, Second Prize in Chemistry. To graduate student Thi Hong Ha Nguyen.

## Trainee Awards (continued)

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- 2018 Illinois Tech Biology/Chemistry/Physics Poster Day, Second Prize. To graduate student Bing Xie.
- 2017 CBSB2017 Outstanding Young Researcher Award. To graduate student Chen Li.
- 2017 Illinois Tech Biology/Chemistry/Physics Poster Day, Second Prize. To graduate student Bing Xie.
- 2017 Kilpatrick Lecture Poster Day, Second Prize. To graduate student Bing Xie.
- 2016 Illinois Tech Biology/Chemistry/Physics Poster Day, Best Chemistry Poster. To senior research associate Trung Hai Nguyen.

## Trainees

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### Visiting scholars

- 2018 M. Reza Gangalikhany, Assistant Professor, Department of Biology, Faculty of Sciences, Isfahan University, Isfahan, Iran.

### Research faculty

- 2020 – 2023 Soohaeng Yoo Willow, Research Assistant Professor.

### Senior research associates

- 2019 – 2020 Soohaeng Yoo Willow. Subsequently, Research Assistant Professor.
- 2019 Chamila Dharawardhana.
- 2019 Bing Xie. Subsequently, postdoctoral researcher at the National Institutes of Health.
- 2014 – 2018 Trung Hai Nguyen. Subsequently, postdoctoral researcher at the University of Illinois, Chicago.
- 2013 – 2016 Laurentiu Spiridon. Subsequently, staff scientist at the Institute of Biochemistry of the Romanian Academy.

### Ph.D. thesis students

- 2024 – present Aiman Khan, Ph.D. in Chemistry.
- 2023 – present Van Anh Tran Nguyen, Ph.D. in Chemistry.
- 2023 – present Yindong Chen, Ph.D. in Applied Mathematics. Secondary advisor, co-advised with Lulu Kang.
- 2022 – present Juan Manuel Meza, Ph.D. in Biology. Secondary advisor, co-advised with Oscar Juarez.
- 2022 – present Jennifer Sorescu, Ph.D. in Biology. Secondary advisor, co-advised with Oscar Juarez.
- 2022 – present Qi Xu, Ph.D. in Chemistry.
- 2020 – present Joseph Depaolo-Boisvert, Ph.D. in Chemistry.
- 2020 – present Van La, Ph.D. in Biology.

## **Trainees (continued)**

- 2020 – present Hong Ha Nguyen, Ph.D. in Chemistry.  
2020 – present James Tufts, Ph.D. in Chemistry.  
2016 – 2019 Xuan Fang, Ph.D. in Biology. Secondary advisor, co-advised with Oscar Juarez.  
2014 – 2018 Bing Xie, Ph.D. in Chemistry. Subsequently, postdoctoral researcher in group.

### **M.S. students**

- 2021 – 2023 Stanley Nicholson, B.S./M.S. in Applied Mathematics. Subsequently, Ph.D. at Brown University.  
2020 – 2022 Tien Do, M.S. in Biology. Primary advisor, co-advised with Oscar Juarez.  
2016 – 2019 William Menzer, B.S./M.S. in Molecular Biochemistry and Biophysics. Primary advisor, co-advised with Oscar Juarez. Subsequently, Ph.D. student at LMU Munich.  
2016 – 2018 Hexi Zhang, M.S. in Chemistry. Subsequently, Ph.D. student with Andrey Rogachev.  
2014 – 2017 Chen Li, M.S. in Chemistry. Subsequently, businessman.

### **Undergraduate honors thesis students**

- 2014 – 2015 Rachael Youngworth, B.S. in Chemistry. Subsequently, Ph.D. student at the University of Chicago.  
2013 – 2015 John Clark, B.S. in Chemistry. Subsequently, Proctor and Gamble.

### **Research Project Students (involved for one or more semesters)**

- 2023 Kevin Alvarado, B.S. in Medicinal Chemistry  
2023 – present David Cooper, B.S. in Medicinal Chemistry  
2023 – present Barien Gad, B.S./M.S. in Biochemistry and Data Science  
2023 – present Prannami Gajjar, M.S. in Data Science  
2023 Beomjong Lee, B.S. in Computer Science  
2023 Urvi Mekala, B.S. in Computer Science  
2023 Poshan Pandey, M.S. in Computer Science  
2023 Thitipun Srinarmwong, M.S. in Computer Science  
2021 – 2022 Amna Haneef, B.S./M.S. in Biology  
2021 – 2022 Kunj Patel, B.S. in Medicinal Chemistry  
2018 – 2019 Natalie “Blaine” Jumonville, B.S. in Physics  
2017 Erica Cusnariov, B.S. in Computer Science  
2017 Robert “Wes” Ludwig, B.S. in Bioinformatics  
2016 – 2017 Kenneth Ford, M.S. in Molecular Biochemistry and Biophysics  
2016 Wenji Sun, M.S. in Biology  
2014 Kyle Burke, Ph.D. in Chemistry  
2014 – 2015 Shubin Zhang, M.S. in Physics

## Trainees (continued)

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2014 – 2015	Yang-Yang Xie, M.S. in Computer Science
2014 – 2015	Yu-Ting Yu, Master of Chemistry

Additionally, I have hosted 24 undergraduate and 11 high school summer interns.

## Courses Taught

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Chem 100	Introduction to the Profession. Spring 2019.
Chem 124	Principles of Chemistry I. Spring 2018.
Chem 343	Physical Chemistry I. Spring 2014, Spring 2016, Fall 2016, Fall 2017, Fall 2018, Spring 2019, Fall 2020, Fall 2021, Spring 2022, Spring 2023.
Chem 484/584/684	Graduate Seminar. Spring 2022.
Chem 485/585/685	Chemistry Colloquium. Spring 2016, Fall 2020, Fall 2021.
Chem 456	Computational Biochemistry and Drug Design. Spring 2020, Summer 2021, Fall 2022.
Chem 460	Bioanalytical Chemistry. Spring 2021.
Chem 550	Chemical Bonding. Fall 2013, Fall 2014, Fall 2015.
Chem 553	Chemical Thermodynamics. Spring 2015, Spring 2017.
I PRO 497	Interprofessional Projects. Fall 2015: User interfaces for novel computer-aided drug design tools; Spring 2016: From physical ball-and-stick to computer models of chemical systems; Summer 2016: An open-source web interface for computer-aided drug design; Spring 2017: Simulating and visualizing moving molecules in biological nanosensors.

## Academic Service

### Internal

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#### Chemistry Department

2023 – present	<b>Member, Biochemistry Collaboration Committee.</b> This joint committee of biology and chemistry faculty manages the interdisciplinary programs.
2022 – 2023	<b>Member, Strategic Plan Committee.</b> This committee developed a strategic plan for the department.
2021	<b>Member, Faculty Search Committee.</b> The committee led the search that culminated in hiring Sameh Elsaidi as an assistant professor.
2020 – present	<b>Director, Bachelor's degree program in Computational Chemistry and Biochemistry.</b>
2019 – present	<b>Member, Graduate Studies Committee.</b> The committee manages the M.S. and Ph.D. programs, including admissions.
2016 – 2022	<b>Member, Undergraduate Programs Committee.</b>



## Internal (continued)

- 2016 **Member, Faculty Search Committee.** The committee led the search that culminated in hiring Jean-Luc Ayitou as an assistant professor.
- 2015 – 2018 **Chair, Ph.D. Qualifying Exam Committee.** Before the exam revision, I coordinated the written exams for M.S. and Ph.D. students. Subsequently, I oversaw the committee that assigns faculty to Ph.D. qualifying exams and addresses exam-related issues.
- 2015 – 2016 **Chair, Graduate Curriculum Revision Committee.** The committee developed and successfully proposed a transition from written exams for M.S. and Ph.D. students to oral exams for Ph.D. students. We also added professional development courses to the non-thesis M.S. program to better prepare students for industry.
- 2014 – 2015 **Member, Undergraduate Curriculum Revision Committee.** The committee reviewed the B.S. curriculum and successfully proposed changes to increase flexibility. We also updated course descriptions and developed documents to improve standardization of classes and laboratories across instructors. I chaired a subcommittee in physical chemistry.
- 2014 **Member, Lecturer Search Committee.** The committee led the search that culminated in hiring Courtney Sobers and Dan Mueller as lecturers.
- 2014 – 2019 **Undergraduate Advising.** I am/have been the academic advisor for 8 chemistry B.S. students. During an associate chair vacancy between Fall 2014 and Spring 2015, I was the lead advisor for the chemistry department.
- 2013 – 2015 **Coordinator, Undergraduate Recruiting.** I worked with the undergraduate admissions office and coordinated faculty participation in recruitment events.
- ### University
- 2020 – present **Member, Interdisciplinary Oversight Committee of the University Faculty Council.**
- 2019 **Member, Kaplan Institute Faculty Innovation Studio.** I represented the chemistry department in a cohort of faculty charged with proposing revisions to the IPRO program and piloting a new type of IPRO offering. The cohort met during the Spring semester.
- 2018 – 2019 **Member, University Research Council.** I represented the chemistry department in matters related to support for research.
- 2018 – present **Associate Director, Center for Interdisciplinary Scientific Computation.** I work with the director to coordinate center activities including seminars and use of a computing cluster.
- 2016 ... **Judge, Illinois Tech Poster Days.** I was a judge at events in 2016 (2), 2017, and 2018, 2021, 2022, and 2023.
- 2014 ... **Interviewer, Camras Scholarship.** I interviewed scholarship finalists in 2014, 2015, and 2017.

## External

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### Event Organization and Judging

- 2022 **Organizer, An International Workshop on Modeling Biological Macromolecules.** I was the main organizer and instructor for a one-week workshop for graduate students and faculty at Simon Bolivar University in Baranquilla, Colombia.
- 2021 **Organizer, An International Workshop on Modeling Biological Macromolecules.** I was the main organizer and instructor for a one-week workshop for advanced undergraduate and early graduate students, primarily from Illinois Tech and Romania.
- 2018 ... **Judge, Chicago Public Schools High School Student Science Fair.** I judged at an event in 2018.
- 2015 **Local Chair, Midwest Enzyme Chemistry Conference.** I coordinated logistics for the annual one-day event with about 200 attendees. It was held at Illinois Tech for the first time.
- 2015 **Organizer, “Choose Your Own Adventure: Solving Real-World Problems with Spectroscopy”.** Along with two other faculty, I developed materials for and coordinated a one-day continuing education workshop for high school science teachers.

### Grant Review

- 2019 **Ad Hoc Reviewer, National Science Centre (Poland).** I reviewed a proposal in 2019.
- 2016 ... **Panelist, National Science Foundation Scientific Review.** I served on one panel in 2016 and one in 2017.
- 2015 ... **Panelist, National Institutes of Health Scientific Review.** I served on one panel in 2015 and one in 2017.
- 2015 ... **Ad Hoc Reviewer, National Science Foundation.** I reviewed proposals in 2015, 2017, 2019, 2020, and 2021.

### Journal Article Review

I have performed over 100 journal article peer reviews. For a verified count of reviews and list of journals, see <https://www.webofscience.com/wos/author/record/596936>.