





Brian D. Nguyen, M.S.

✉ bdnnguye2@uci.edu


in brian-nguyen

Education




- Sept 2016 – exp. Jun 2022  **Ph.D. University of California, Irvine** in Computational and Theoretical Chemistry.
Thesis title: *Understanding the Behaviors of Dispersion Interactions.*
- Sept 2016 – Jun 2021  **M.S. University of California, Irvine** in Chemical and Materials Physics.
- Sept 2011 – Mar 2015  **B.S. University of California, Irvine** in Chemistry, *cum laude*.
-  **B.S. University of California, Irvine** in Biological Sciences, *cum laude*.

Research Experience




Graduate

- Sept 2016 – present  **University of California, Irvine** - Irvine, CA. *Graduate Researcher, Chemistry*
Advisor: Filipp Furche
- Theory and Development**
- Derived and developed the adiabatic connection symmetry adapted perturbation theory (AC-SAPT) to understand the behaviors of noncovalent interactions (NIs)
 - Applied AC-SAPT framework to diagnose and determine computational methods that can accurately predict NIs
 - Developed multivariate AC-SAPT framework establishing the dispersion size-consistency condition
- Application-based projects**
- Communicated with experimentalists from the Vanderwal Lab at UCI and modelled the ~200,000 atoms ribosome-drug interaction via *in silico* which has led to potential drug candidates; publication *in prep*
 - Provided computational models for Long Group at UC Berkeley to understand the electronic structure of dilanthanide single molecule magnets; published in *J. Am. Chem. Soc.*
 - Developer for the TURBOMOLE quantum package suite and collaborated with TURBOMOLE developers worldwide via Git version control
 - Contributed code that analyzes the density errors of electronic structure methods





Undergraduate

- Jun 2015 - Sept 2015  **University of California, Irvine** - Irvine, CA. *Undergraduate Researcher, Mathematics*
Advisor: Frederic Y. Wan
- 1 of 20 students accepted into the Mathematical and Computational Biology for Undergraduate summer program
 - Engaged with mathematician to develop a dynamic kinetic model that predicted the early development of fruit flies matching experimental studies
- Mar 2014 - Jun 2016  **University of California, Irvine** - Irvine, CA. *Undergraduate Researcher, Biology*
Advisor: Thomas L. Poulos
- Simulated and predicted the mechanism of *Leishmania major* peroxidase through molecular dynamics (MD) simulations; results supported experiments and published in *J. Chem. Info. Model.*
 - Predicted the dominant protein conformation of cytochrome P450 through MD simulations matching experiments; published in *Proc. Natl. Acad. Sci. U.S.A.*
- Oct 2013 - Jun 2016  **University of California, Irvine** *Undergraduate Researcher, Chemistry*
Advisor: Filipp Furche
- Supported Prescher Lab with computational models to produce luciferin derivatives that emit ~2x stronger signal for bioluminescence; published in *ChemBioChem*
 - Developed up to ~4x faster algorithm for molecular property in the excited state and contributed code to the TURBOMOLE quantum package; published in *J. Chem. Phys.*

Work Experience




- Jan 2019 – Mar 2019  **University of California, Irvine** - Irvine, CA. *Graduate Chemistry Teacher Assistant*
- Taught for two graduate level chemistry courses: Chem 254 - Computational Chemistry and Chem 232B - Quantum Mechanics
 - Facilitated discussion utilizing weekly worksheets and guided computational lab sections for over 40 students
- Sept 2016 – Jun 2017  **University of California, Irvine** - Irvine, CA. *Undergraduate Chemistry Teacher Assistant*
- Taught for general chemistry lecture and lab courses (Chem M2LA/H2LA, Chem 1B, and Chem 1C)
 - For over 200 students, directed and encouraged small group work in discussion sections
 - Guided and supervised over 40 students in lab sections
- Dec 2015 – Jun 2016  **Morpho Detection, LLC** - Santa Ana, CA. *Chemist Intern*
- Tested the accuracy of mass spectrometry device for bomb detection and communicated with senior scientists on the development of the devices
 - Calibrated and tested the bomb detection accuracy of the devices for government certification

Mentoring Experience

- Sept 2016 – present  **Furche High School Outreach Program** - Irvine, CA.
- Led the outreach program to provide research opportunities for underserved communities throughout the United States
 - Cultivated a community of 21 high school students and 12 graduate mentors
 - Volunteered 5000+ hours and co-authored National Science Foundation research grant to support the program
 - Provided weekly one-on-one research mentorship for 4 high school students (Matthew Tang, Jenny Nguyen, Thanh Huynh, and Natalie Tran)
 - Jenny, Matthew, and Thanh are pursuing biology, earth system science, and chemistry majors, respectively, at University of California campuses
- Sept 2017 – present  **UCI Undergraduate Research Mentorship** - Irvine, CA
- Mentored and performed research alongside 4 first generation undergraduates (Emily Barragan, Poorvi Rao, Devin J. Hernandez, and Emmanuel V. Flores)
 - Emily is pursuing Chemical Engineering Ph.D. program at Columbia University and Devin has been accepted to Chemistry Ph.D. program at University of California, Berkeley
- Jun 2017 – Sept 2017  **UCI Competitive Edge Peer Mentor** - Irvine, CA.
- Welcomed incoming UCI doctoral students for smooth transition into graduate school
 - Provided weekly one-on-one individual meetings for mentees to discuss research, presentation skills, and fellowship applications
- Sept 2016 – Feb 2020  **Orange County Regional Science Olympiad** - Irvine, CA.
- Created and standardized 8 experimental design exams for middle and high school students in 2017, 2018, 2019, and 2020 OC Regional Science Olympiad at UCI
 - Mentored and taught an undergraduate to design and proctor the experimental design exam

Publications

Journal Articles

- 1 **Nguyen, B.D.***, Hernandez, D.J.*, Flores, E. V., & Furche, F. (2022). Dispersion size-consistency. *Electron. Struct.*, 4(1).  doi:10.1088/2516-1075/ac495b
- 2 Darago, L. E., Boshart, M. D., **Nguyen, B.D.**, Perl, E., Ziller, J. W., Lukens, W. W., ... Long, J. R. (2021). Strong ferromagnetic exchange coupling and single-molecule magnetism in MoS_4^{3-} -bridged dylanthanide complexes. *J. Am. Chem. Soc.*, 143(22), 8465–8475.  doi:10.1021/jacs.1c03098
- 3 Yu, J.M.*, **Nguyen, B.D.***, Tsai, J., Hernandez, D. J., & Furche, F. (2021). Selfconsistent random phase approximation methods. *J. Chem. Phys.*, 155(4), 040902.  doi:10.1063/5.0056565

- 4 Balasubramani, S. G., Chen, G. P., Coriani, S., Diedenhofen, M., Frank, M. S., & [Nguyen, B.D. and including 29 others]. (2020). Turbomole: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. *J. Chem. Phys.*, 152(18), 184107. [doi:10.1063/5.0004635](#)
- 5 Nguyen, B.D., Chen, G. P., Agee, M. M., Burow, A. M., Tang, M. P., & Furche, F. (2020). Divergence of many-body perturbation theory for noncovalent interactions of large molecules. *J. Chem. Theory Comput.*, 16(4), 2258–2273. [doi:10.1021/acs.jctc.9b01176](#)
- 6 Hollingsworth, S.A.* and Nguyen, B.D.*, Chreifi, G., Arce, A. P., & Poulos, T. L. (2017). Insights into the dynamics and dissociation mechanism of a protein redox complex using molecular dynamics. *J. Chem. Inf. Model.*, 57(9), 2344–2350. [doi:10.1021/acs.jcim.7b00421](#)
- 7 Steinhart, R. C., Rathbun, C. M., Krull, B. T., Yu, J. M., Yang, Y., Nguyen, B.D., ... Prescher, J. A. (2017). Brominated luciferins are versatile bioluminescent probes. *ChemBioChem*, 18(1), 96–100. [doi:10.1002/cbic.201600564](#)
- 8 Furche, F., Krull, B. T., Nguyen, B.D., & Kwon, J. (2016). Accelerating molecular property calculations with nonorthonormal krylov space methods. *J. Chem. Phys.*, 144(17), 174105. [doi:10.1063/1.4947245](#)
- 9 Hollingsworth, S.A.* and Batabyal, D.* , Nguyen B.D., & Poulos, T. L. (2016). Conformational selectivity in cytochrome p450 redox partner interactions. *Proc. Natl. Acad. Sci. U.S.A.*, 113(31), 8723–8728. [doi:10.1073/pnas.1606474113](#)

* Indicates authors contributed equally to the publication

Presentations

- 1 Nguyen, B.D., Hernandez, D. J., Flores, E. J., & Furche, F. (2022). Dispersion size-consistency within the adiabatic connection symmetry-adapted perturbation theory. Oral. 2022 Spring ACS National Meeting & Expo. San Diego, CA.
- 2 Nguyen, B.D., Chen, G. P., Agee, M. M., Burow, A. M., & Furche, F. (2020). Divergence of many-body perturbation theory. Poster. 2020 Fall ACS National Meeting & Expo. San Francisco, CA.
- 3 Nguyen, B.D., Chen, G. P., Agee, M. M., Burow, A. M., & Furche, F. (2019). Size dependence of noncovalent interactions within rpa. Poster. 2019 Southern California Theoretical Chemistry Symposium. Los Angeles, CA.
- 4 Nguyen, B.D., Chen, G. P., Agee, M. M., Burow, A. M., & Furche, F. (2018). Accuracy of rpa for large weakly interacting systems. Poster. 2018 Conference on Excited States Processes. Santa Fe, NM.



Invited Talk

- 1 Nguyen, B.D., Chen, G. P., Agee, M. M., Burow, A. M., Tang, M., & Furche, F. (2021). *Are dispersion interactions weak?* University of Vienna, Vienna, Austria.

Awards and Certifications

Feb 2022	 UCI Grad Slam Semifinalist University of California, Irvine
Jun 2021	 UCI School of Physical Sciences Faculty Endowed Fellowship University of California, Irvine  UCI Dissertation Fellowship in Chemistry University of California, Irvine
Sept 2016	 UCI Graduate Chancellor Fellowship in Chemistry University of California, Irvine
Jun 2015	 UCI Chancellor's Undergraduate Award of Distinction University of California, Irvine
May 2015	 Phi Beta Kappa  Phi Lambda Upsilon
Jun 2014	 Hypercube Scholar Award Hypercube Inc.
Apr 2014	 OC American Chemical Society Undergraduate Award Orange County American Chemical Society Local Chapter

Certifications

Mar 2020	 UCI Graduate Division Mentoring Excellence Program
Jun 2017	 UCI GPS-BIOMED Effective Communication Program