





# Brian D. Nguyen, M.S.

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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
- 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. *Elec. 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  $\text{MoS}_4^{3-}$ -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	 <b>UCI Grad Slam Semifinalist</b> University of California, Irvine
Jun 2021	 <b>UCI School of Physical Sciences Faculty Endowed Fellowship,</b> University of California, Irvine  <b>UCI Dissertation Fellowship in Chemistry,</b> University of California, Irvine
Sept 2016	 <b>UCI Graduate Chancellor Fellowship in Chemistry,</b> University of California, Irvine
Jun 2015	 <b>UCI Chancellor's Undergraduate Award of Distinction,</b> University of California, Irvine
May 2015	 <b>Phi Beta Kappa</b>  <b>Phi Lambda Upsilon.</b>
Jun 2014	 <b>Hypercube Scholar Award,</b> Hypercube Inc.
Apr 2014	 <b>OC American Chemical Society Undergraduate Award,</b> Orange County American Chemical Society Local Chapter

## Certifications

Mar 2020	 <b>UCI Graduate Division Mentoring Excellence Program</b>
Jun 2017	 <b>UCI GPS-BIOMED Effective Communication Program</b>