# Brian D. Nguyen, Ph.D.
bdnguye2@uci.edu
brian-nguyen

## Education

Sept 2016 – *exp.* Jun 2022 — **Ph.D. University of California, Irvine** in Computational and Theoretical Chemistry.
Thesis title: *Understanding the Behavior 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

Sept 2016 - present — **University of California, Irvine** - Irvine, CA. *Graduate Researcher, Chemistry*
Advisor: Filipp Furche

- Developed theories and models to predict the behavior of noncovalent interactions
- Initiated cancer drug collaboration with the Vanderwal Lab at UCI and developed model of the ∼200,000 atoms protein-drug complex leading to potential drug candidates; publication *in prep*
- Collaborated with the Long Group at UC Berkeley and developed model to understand the electronic structure of dilanthanide single molecule magnets; published in *J. Am. Chem. Soc.*
- Provided weekly one-on-one research mentorship for 4 undergraduates and 4 high school students
- 1 undergraduate pursued Chemical Engineering Ph.D. program at Columbia University and 4 high school students pursued biology, earth system science, and chemistry majors at UCI and UCSB

Jun 2016 - Sept 2016 — **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
- Collaborated with mathematician to develop a mathematical 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 *PNAS*

Oct 2013 - Jun 2016 — **University of California, Irvine** *Undergraduate Researcher, Chemistry*
Advisor: Filipp Furche

- Collaborated with Prescher Lab to produce luciferin derivatives that emit ∼2x stronger signal for bioluminescence; published in *ChemBioChem*
- Developed up to ∼4x faster algorithm for molecular property calculations and coded within 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
- Led discussion and 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)
- Led discussion and lab sections for over 200 students

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

## Publications

### Journal Articles

1. **Nguyen, B.**, Hernandez, D. J., Flores, E. V. V., & Furche, F. (2022). Dispersion size-consistency. *Elec. Struct.* doi:10.1088/2516-1075/ac495b
2. Darago, L. E., Boshart, M. D., **Nguyen, B.D.**, Perlt, E., Ziller, J. W., Lukens, W. W., … Long, J. R. (2021). Strong ferromagnetic exchange coupling and single-molecule magnetism in $MoS_4^{3-}$-bridged dilanthanide 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., Franzke, Y. J., … Yu, J. M. (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., **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. Steinhardt, 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., 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

## Presentations

1. **Nguyen, B.D.**, Hernandez, D. J., Flores, E. J., & Furche, F. (2021). Dispersion size-consistency. *accepted* Oral. 2021 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.

## Skills

Programming — C++, Fortran, bash, Python, R, MATLAB, LaTeX

## Miscellaneous Experience

### Extracurriculars

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; created a community with 18 high school students and 10 graduate mentors
- Volunteered 5000+ hours and co-authored research grants to support the program

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

### Awards and Achievements

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**