





Brian D. Nguyen, Ph.D.

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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 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


Graduate

- 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.*
 - Developer for the TURBOMOLE quantum package suite and contributed to the code



Undergraduate

- 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

Work Experience (continued)







- 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




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; created a community with 18 high school students and 10 graduate mentors
 - Volunteered 5000+ hours and co-authored research grants to support the program
 - Provided weekly one-on-one research mentorship for 4 high school students (Matthew, Jenny, Thanh, and Natalie)
 - Mentees are pursuing biology, earth system science, and chemistry majors at UCI and UCSB
- Sept 2017 – present  **UCI Undergraduate Research Mentorship** - Irvine, CA
- Mentored and performed research alongside 4 undergraduates (Emily, Poorvi, Devin, and Emmanuel)
 - Emily pursued Chemical Engineering Ph.D. program at Columbia University and Devin has been accepted to
- 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.**, Hernandez, D. J., Flores, E. V. 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 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., 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. (2022). Dispersion size-consistency. *accepted* 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.

Skills

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

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