Brian D. Nguyen, Ph.D.
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brian-nguyen

Education

Sept 2016 – Jun 2022 — **Ph.D. University of California, Irvine** in Computational and Theoretical Chemistry.
Thesis title: *Developing the Theory of Dispersion Interactions for Biological Applications.*

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.**, 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., & [**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. 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.* 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**