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Education

Ph.D Chemistry (Anticipated May 2022) Advisor: Filipp Furche University of California, Irvine	2016-Present
B.S. Chemistry, B.S. Biology University of California, Irvine	2011-2015

Publications

1. **Nguyen, B.D.**[†]; Hernandez, D.J.[†]; Flores, E.; Furche, F. Dispersion Size-Consistency. *Under Review*. **2021**.
2. **Nguyen, B.D.**[†]; Yu, J.M.[†]; Tsai, J.; Furche, F. Selfconsistent Random Phase Approximation Methods. *J. Chem. Phys.* **2021**, *155*(4), 040902.
3. Darago, L.E.; Boshart, M.D.; **Nguyen, B. D.**; Perlt, E.; Ziller, J.W.; Lukens, W.W.; Furche, F.; Evans, W.J.; Long, J.R. Strong Ferromagnetic Exchange Coupling and Single-Molecule Magnetism in MoS₄³⁻-Bridged Dilanthanide Complexes. *J. Am. Chem. Soc.* **2021**, *143*(22), 8465–8475.
4. Balasubramani, S.G.; [and 36 others, including **Nguyen, B.D.**] TURBOMOLE: Modular Program Suite for Ab Initio Quantum-Chemical and Condensed-Matter Simulations. *J. Chem. Phys.* **2020**, *152*(18), 184017.
5. **Nguyen, B.D.**; Chen, G.P.; Agee, M.M.; Burow, A.M.; Tang, M.P.; Furche, F. Divergence of Many-Body Perturbation Theory for Noncovalent Interactions of Large Molecules. *J. Chem. Theory Comput.* **2020**, *16*(4), 2258–2273.
6. **Nguyen, B.D.**[†]; Hollingsworth, S.A.[†]; Chreifi, G.; Arce, A.P.; Poulos, T.L. Insights into the Dynamics and Dissociation Mechanism of a Protein Redox Complex Using Molecular Dynamics. *J. Chem. Info. Model.* **2017**, *57*(9), 2344–2350.
7. Steinhardt, R. C.; Rathbun, C.M.; Krull, B.T.; Yu, J.M.; Yang, Y.; **Nguyen, B.D.**; Kwon, J.; McCutcheon, D.C.; Jones, K.A.; Furche, F.; Prescher, J. A. Brominated Luciferins Are Versatile Bioluminescent Probes. *ChemBioChem* **2016**, *18*(1), 96–100.

8. Hollingsworth, S. A.[†]; Batabyal, D.[†]; **Nguyen, B. D.**; Poulos, T. L. Conformational Selectivity in Cytochrome P450 Redox Partner Interactions. *Proc. Natl. Acad. Sci.* **2016**, *113*(31), 8723–8728.
9. Furche, F.; Krull, B.T.; **Nguyen, B.D.**; Kwon, J. Accelerating Molecular Property Calculations with Nonorthonormal Krylov Space Methods. *J. Chem. Phys.* **2016**, *144*(17), 174105.

[†] Indicates that authors contributed equally

Research Experience

Graduate Researcher, Chemistry 2017-Present

University of California, Irvine

Advisor: Filipp Furche

Research: Understanding the behavior of noncovalent interactions, and mentoring 15 high school and 4 undergraduate students.

Undergraduate Researcher, Mathematics Summer 2016

University of California, Irvine

Advisor: Frederic Y. Wan

Research: Developed mathematical model of the early development of fruit fly.

Undergraduate Researcher, Biology 2014-2016

University of California, Irvine

Advisor: Thomas L. Poulos

Research: Simulated mechanism of *Leishmania major* peroxidase, and predicted the dominant protein conformation of cytochrome P450.

Undergraduate Researcher, Chemistry 2013-2016

University of California, Irvine

Advisor: Filipp Furche

Research: Developed luciferin derivatives for bioluminescence, and improved molecular property calculations for TURBOMOLE quantum package.

Selected Poster Presentations

2020 Fall ACS National Meeting & Expo, *San Francisco*, Poster.

Nguyen, B.D.; Chen, G.P.; Agee, M.M.; Burow, A.M.; Tang, M.P.; Furche, F. Divergence of Many-Body Perturbation Theory, April **2020**,

2019 Southern California Theoretical Chemistry Symposium, *Los Angeles*, Poster.

Nguyen, B.D.; Chen, G.P.; Agee, M.M.; Burow, A.M.; Furche, F. Size dependence of noncovalent interactions within RPA, May **2019**
