Matthew J. Varga
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Profile

- Ph.D. computational chemist with ~1.5 years of postdoctoral experience at Johns Hopkins University.
- Interdisciplinary educational and research background in physical chemistry, biochemistry, and biophysics.
- 3 first author or co–first author papers, such as in the *Journal of Chemical Theory and Computation*.
- 5+ years experience in utilizing molecular dynamics and Monte Carlo methods to study biological systems.
- Proficient in the use of C++ and Python for scientific software development and data analysis.

Education

- **Doctor of Philosophy in Chemistry** 2012 - 2017
  University of Arizona *Tucson, AZ*
  - Adviser: Dr. Steven D. Schwartz
  - Dissertation: The Dynamics of Dehydrogenases – A Phase Space Odyssey
- **Bachelor of Arts in Chemistry** 2009 - 2012
  College of Wooster *Wooster, OH*
  - Senior Thesis: Functionalized Swellable Glass as a Catalyst Support for Suzuki-Miyaura Coupling Reactions
  - Transferred from University of Puget Sound (attended 2008–2009).

Research Experience

- **Postdoctoral Research Fellow** August 2017 - Present
  Johns Hopkins University, Department of Biophysics *Baltimore, MD*
  - Principal Investigator: Dr. Margaret Johnson
  - Developing and utilizing stochastic simulation methods for studying biological self–assembly with single–particle and temporal resolution. Focus on software and algorithm development.
  - Automated and manual data curation of protein–protein interaction networks.
  - Determining, *in silico*, dissociation constants of dimerization for membrane curvature–inducing proteins, using coarse–grained molecular dynamics and enhanced sampling (metadynamics).
- **Graduate Research Assistant** January 2013 - July 2017
  University of Arizona, Department of Chemistry and Biochemistry *Tucson, AZ*
  - Principal Investigator: Dr. Steven D. Schwartz
  - Examined the chemistry of enzymatic reactions, specifically the relationship between structure and dynamics in dehydrogenases, using molecular dynamics and Monte Carlo methods.
  - Utilized a previously developed algorithm to calculate kinetic isotope effects of enzymatic reactions from first principles, and applied it to hydride transfer in yeast alcohol dehydrogenase. This work also utilized algorithms to include the effects of quantum tunneling into molecular dynamics simulations.
  - Studied two independently evolved lactate dehydrogenases, from two *Apicomplexa* organisms, to determine how catalytically important dynamics change with alterations to secondary structure near the active site.
- **Undergraduate Research Assistant** August 2009 - May 2012
  College of Wooster, Department of Chemistry *Wooster, OH*
  - Principal Investigator: Dr. Paul Edmiston
  - Developed sol-gel materials for use in ground water remediation and as catalysts for organic reactions, such as the Suzuki-Miyaura reaction. Culminated in a senior independent study thesis.

Skills

Methods: Molecular dynamics, high performance computing, stochastic simulations, enhanced sampling methods, semi-classical and *ab–initio* quantum methods, Monte Carlo

Scientific Packages: CHARMM, Gromacs, Gaussian, VMD, PyMol

Programming Languages: C++, Python

Operating Systems: Linux/Unix, macOS, Windows

References

Dr. Margaret Johnson (*margaret.johnson@jhu.edu* | 410-516-2376). Assistant Professor of Biophysics, Johns Hopkins University.

Dr. Steven D. Schwartz (*sschwartz@email.arizona.edu* | 520-621-6363). Professor of Chemistry and Biochemistry *and* of Applied Mathematics, University of Arizona.

Dr. Andrei Sanov (*sanov@email.arizona.edu* | 520-626-4361). Professor of Chemistry and Biochemistry *and* of Physics, University of Arizona.

Teaching Experience

- **Graduate Teaching Assistant** Fall 2012, Spring 2016, Spring 2017
  University of Arizona, Department of Chemistry and Biochemistry *Tucson, AZ*
  - Taught two sections of General Chemistry laboratory consisting of 24 students each. Responsibilities included lecturing on general chemistry concepts, teaching proper laboratory skills and safety, and monitoring students as they performed experiments.

Publications

Varga, M.J.; Dzierlenga, M.W.; Schwartz, S.D. Structurally Linked Dynamics in Lactate Dehydrogenases of Evolutionarily Distinct Species. *Biochemistry* 2017, 56, 2488–2496.

Dzierlenga, M.W.*; **Varga, M.J.***; Schwartz, S.D. Path Sampling Methods for Enzymatic Quantum Particle Transfer Reactions. In *Methods in Enzymology*; 2016; Vol. 578, pp 21–43.

* *Co-first author*

Varga, M.J.; Schwartz, S.D. Enzymatic Kinetic Isotope Effects from First Principles Path Sampling Calculations. *J. Chem. Theory Comput.* 2016, 12 (4), 2047–2054.

Select Presentations

Varga, M.J. "Dynamics of Dehydrogenases – A Phase Space Odyssey." Lectures in Computational Biophysics, Johns Hopkins University. Baltimore, MD. Feb. 13th, 2018.

Varga, M.J. "Evidence for evolutionary change in the way protein dynamics contributes to enzyme catalysis." University of Arizona Department of Chemistry and Biochemistry. Tucson, AZ. Nov. 14th, 2016.

Varga, M.J. "Determination of enzymatic kinetic isotope effects in yeast alcohol using transition path sampling." American Physical Society Spring Meeting. San Antonio, TX. Mar. 2nd, 2015.

Varga, M.J. "Determination of enzymatic kinetic isotope effects in yeast alcohol using transition path sampling." University of Arizona Department of Chemistry and Biochemistry. Tucson, AZ. Feb. 16th, 2015.

Varga, M.J. "Using Transition Path Sampling to Determine the Rate of Hydride Transfer in Yeast Alcohol Dehydrogenase." University of Arizona Department of Chemistry and Biochemistry. Tucson, AZ. Oct. 14th, 2013.

Departmental Activities

Admissions and Recruiting Committee (University of Arizona, Department of Chemistry and Biochemistry)

Affiliations

American Chemical Society, American Physical Society, Biophysical Society