# Robert M. Raddi

Ph.D. Candidate in Theoretical Chemistry

### Summary

I'm a theoretical chemist from the greater Philadelphia area who loves experiencing diverse cultures, meeting new people, hiking, and programming. The broad view of my research focuses on developing scientific software packages that use machine learning/physics based approaches to tackle problems in chemistry and structural biology.

# robraddi.github.io

n Philadelphia, PA 267-312-0604

mraddi@temple.edu



github.com/robraddi



in linkedin.com/in/rraddi



#### **Publications**

- 1. Raddi, Robert, and Vincent Voelz. "Stacking Gaussian Processes to Improve pKa Predictions in the SAMPL7 Challenge." (2021).
- 2. Voelz, Vincent A., Yunhui Ge, and Robert M. Raddi. "Reconciling simulations and experiments with BICePs: a review." Frontiers in Molecular Biosciences 8 (2021): 325.
- 3. Robert M. Raddi, Yunhui Ge, and Voelz, Vincent A. "BICePs 2.0: new tools for Bayesian Inference of Conformational Populations from Theory and Experiment." submitted
- 4. Robert M. Raddi, Tim Marshall, Yunhui Ge, and Voelz, Vincent A. "BICePs RepX: Force Field Validation by Bayesian Inference."

in preparation

5. Robert M. Raddi, Richard Baxter, and Voelz, Vincent A. "Reconciling simulated ensembles of Serotransferrin with experimental SAXS intensities." in preparation

# **Experience**

# 2021

Jan. - Dec. Research Assistant

Award: 1st place poster presentation at ACS EUS YCC Research Symposium

2020

Jan. - Dec. Research Assistant/Teaching Assistant

TA Assignments: Physical Chemistry of Biomolecules & Techniques of Chemical Measurement II

2019

Jan. - Dec. Research Assistant/Teaching Assistant

TA Assignments: Physical Chemistry of Biomolecules, Chemistry for Engineers recitation, General Chemistry I laboratory, General Chemistry II laboratory

**Award:** The Guy Allen Award for Outstanding Teaching **Certification:** Teaching in Higher Education Certificate Extra: Acedemic Intern for Computing & Statistics Summer Workshop, Temple University Physics Department

2018

Sept. - Dec. Research Assistant/Teaching Assistant

TA Assignments: General Chemistry I recitation & laboratory

#### **Education**

## Ph.D. Candidate in Chemistry

Advisor: Dr. Vincent Voelz Temple University Philadelphia, PA 2018 - 2023 (expected)

#### **B.S in Chemistry**

Temple University Philadelphia, PA 2013 - 2017

#### **Skills**

- GNU/Unix & HPC
- Software/Package Development
- Python, C/C++, Cython, Bash
- LaTex, HTML/CSS, Markdown
- MD Simulations (Gromacs & OpenMM)
- MCMC Simulations
- Molecular Modelling
- Cheminformatics
- Bayesian Inference & Statistical Inference
- Machine Learning
- Scientific Communication
- Teaching