# Robert M. Raddi

Ph.D. Candidate in Theoretical Chemistry

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🔷 Robert Raddi

## Summary

I am a 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 physics/machine learning based approaches to tackle problems in chemistry and structural biology.

## Publications

1. **Raddi, Robert**, and Vincent Voelz. "Stacking Gaussian Processes to Improve pKa Predictions in the SAMPL7 Challenge."Journal of Computer-Aided Molecular Design 35 (2021): 953-961.
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." **(to be submitted)**
4. **Robert M. Raddi**, Tim Marshall, Yunhui Ge, and Voelz, Vincent A. "BICePs RepX: Force Field Validation by Bayesian Inference." **(in revising stage)**
5. **Robert M. Raddi**, Richard Baxter, and Voelz, Vincent A. "Reconciling simulated ensembles of Serotransferrin with experimental SAXS intensities." **(in research stage)**

## 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

## Experience

**2021**

**Jan. — Dec.** Research Assistant

**Award:** 1st Place Poster Presentation at ACS EUS YCC Research Symposium "Reconciling Simulations and Experiments With BICePs"

**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
**Outreach:** Student Mentor for New Foundations Charter School

## 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