Shane W. Flynn

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Education

Ph.D Theoretical Chemistry, University of California Irvine. Irvine, CA, USA 2017-2021
Research Advisor: Vladimir A. Mandelshtam (Expected)

M.S. Theoretical Chemistry, California Institute of Technology. Pasadena, CA, USA 2015-2017
Research Advisor: William A. Goddard III

B.S. Chemistry. B.S. Biology., University of Massachusetts Boston. Boston, MA, USA 2010-2015
Research Advisors: Jason R. Green. Steven M. Ackermann

Research Experience

Quasi-Regular sampling of any distribution function Jan 2017-Present

- Derived and implemented a general sampling method generating points that are locally uniform, and sample the global distribution.
- Derived and implemented a Distributed Gaussian Basis to compute the RoVibrational spectra for a given chemical system.
- Quantitatively demonstrated the superior efficiency of QRGs compared to known methods such as metropolis Monte Carlo, and quasi-Monte Carlo.

Thermodynamic analysis of polymer electrolytes for battery applications 2015-2017

- Developed a computational screening paradigm to search for potential polymer electrolytes for battery applications.
- Extended the use of the Two-Phase Thermodynamic model to study polymer thermodynamics independent of potential ions, greatly reducing the complexity associated with candidate screening.

Quantifying disorder present in irreversibly decaying chemical processes 2012-2015

- Developed a new framework in chemical kinetics, resulting in a quantitative measurement for the cumulative fluctuations that occur in rate coefficients.
- Derived a relationship between the rate coefficients found in chemical kinetics to the Fisher Information from information theory.

Publications

- **Shane W. Flynn**, Vladimir Mandelshtam. "Sampling general distributions with quasi-regular grids: Application to the vibrational spectra calculations".
- Jonathan W. Nichols, **Shane W. Flynn**, Jason R. Green. "Order and disorder in irreversible decay processes".
- **Shane W. Flynn**, Helen C. Zhao, Jason R. Green. "Measuring disorder in irreversible decay processes".

Teaching Experience (Teaching Assistant)

- **Mathematical Methods in Chemistry** 2020
  Graduate Level,Ch.237. University of California, Irvine.
- **Thermodynamics and Introduction to Statistical Mechanics** 2019
  Graduate Level,Ch.232A. University of California, Irvine.
- **Nature of the Chemical Bond** 2016
  Graduate Level, Ch.120A. California Institute of Technology, Pasadena.
- **Linear Algebra** 2014
  Undergraduate Level, Ma.260. University of Massachusetts, Boston.