Shane W. Flynn

shane.flynn001@gmail.com   (413)-841-5470
swflynn@uci.edu   LinkedIn: https://www.linkedin.com/in/shane-flynn-676b72184/

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. Minor Mathematics, 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. "Molecular spectra calculations using an optimized quasi-regular Gaussian basis and the collocation method." (accepted)
- **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)

- **Numerical and Mathematical Methods**   2020
  Graduate Level,Ch.237. University of California, Irvine.
- **Thermodynamics and 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.