

Shane W. Flynn

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Medical Engineering
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Experience

Sampling a general distribution function using Quasiregular Grids. Jan 2019-2020

- Developed a novel method for efficient sampling of a general multi-dimensional distribution function.
- Implementation for either Fortran or Python sampling model potentials.
- Applications to vibrational spectra calculations using distributed Gaussian basis sets to solve the generalized eigenvalue problem.
- **Shane W. Flynn**, Vladimir A. Mandelshtam, “Sampling general distributions with quasi-regular grids: Application to the vibrational spectra calculations” *J. Chem. Phys. Comm.* **2019** 151(24) p.241105
- https://github.com/swflynn/Quasi-Regular_Grids

Skills

Programming Languages: Python, Fortran, Java

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, Biology. Minor Math, University of Massachusetts, Boston, Boston MA 2010-2015
Research Advisors: Jason R. Green, Steven A. Ackermann