JOSHUA J. GOINGS, PH.D.

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SKILLS

Programming	Python, Bash, Git, SQL, C++, LaTeX
Data Science	Pandas, Numpy, Matplotlib, Scikit-learn, Keras/Tensorflow, Machine learning, Statistics, Bokeh
Computing	High-performance computing (HPC), OpenMP, Command-line (Linux/Unix)

EXPERIENCE

Yale University, New Haven, CT — 2018–present

Postdoctoral Research Associate

- Created explainable machine learning models to identify crucial molecular motions that influence reaction dynamics relevant to the design of artificial photosynthetic systems (Python, Keras/Tensorflow).
- Built statistical models of photoactive proteins from time-series data to predict protein conformational probabilities.
- Developed and taught a new computational chemistry course at Yale for both graduate and undergraduate students. Designed hands-on exercises and demonstrations to make computational chemistry and high-performance computing broadly accessible to students of all levels and backgrounds, earning a 4.7/5.0 on student evaluations.
- Secured a total of 10.5M CPU-hours (∼$525k value) at the San Diego Supercomputing Center over three years time by writing concise yearly proposals to convey project impact, justify resource use, and substantiate progress to date.
- Published 26 peer-reviewed publications and presented results to international experts at nine conferences.
- Advised and personally mentored multiple graduate students in novel projects in computational biophysics.

University of Illinois, Urbana-Champaign, IL — 2017–18

Postdoctoral Research Associate (team acquired by Yale in 2018)

- Led the theoretical efforts alongside an international team of experimental researchers to provide computational models to predict and control chemical reactivity in artificial photosynthetic systems.
- Applied enhanced-sampling molecular dynamics to predict and observe rare events in a photoactive protein relevant to optogenetics. Wrote statistical analyses to quantitatively predict real-world experimental data.

University of Washington, Seattle, WA — 2012–17

NSF Graduate Research Fellow

- Developed algorithms to simulate the dynamics of electrons in molecules. The methods are available in the open-source software package ChronusQuantum (C++).
- Implemented an efficient algorithm to predict how molecules interact with light. This method is an order of magnitude faster than previous approaches and is available in the commercial software package Gaussian16 (Fortran).
- Spearheaded the computational operations alongside a team of experimental researchers to demonstrate the first 3D imaging of "excited" nanoscale quantum dots (`https://phys.org/news/2018-02-d-imaging-quantum-dots.html`).

EDUCATION

University of Washington, Seattle, WA — 2017

Ph.D. Theoretical (Computational) Chemistry

Seattle Pacific University, Seattle, WA — 2012

B.S. Chemistry & Biochemistry