Christian Venturella

Ph.D. Student - Theoretical Chemistry, Yale University, New Haven, CT

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website - github - LinkedIn

Institutions

Ph.D. Student, Theoretical Chemistry, *Yale University* SEP 2022 — CURRENT
Bachelors in Chemistry, *Princeton University* SEP 2017 — MAY 2021
Program in Applied and Computational Mathematics
Program in Applications of Computing
Program in Materials Science and Engineering

Awards and Honors

Graduate Awards
- NDSEG Fellowship 2024
- NSF GRFP Fellowship Awardee 2024

Undergraduate Awards
- summa cum laude (2021)
- American Institute of Chemists Student Award (2021)
- Sigma Xi Research Society (2021)
- Fulbright Semifinalist (2021)

Research and Work Experience

Ph.D. Research / Theoretical Chemistry **AUG 2022 — CURRENT**
The Zhu Group *Yale University, New Haven, CT*
- Formulated machine learning method for predicting many-body quantum chemistry
- Constructed symmetry adapted intrinsic atomic orbital basis transformations for modeling quantum many body properties in a local orbital representation
- Generated and maintained a database of 10,000+ GW and coupled cluster simulations in massively parallel fashion for molecular and nanomaterial systems
- Engineered workflow for extracting photoemission spectrum, density matrix, energy, and excited states from imaginary-freqeuncy self-energy ML predictions
- Developed graph attention network architectures for predicting many-body physics by targeting the self-energy over DFT orbital graphs. Achieved improved performance, heightened data efficiency, and improved generalizability over existing methods on similar benchmarks.

Software Engineering and Data Science / Educational Data Analytics **JUL 2021 — JUL 2022**
LinkIt! *New York City, NY*
- Engineered a data analysis system for generation of regular administrative reports in PDF and web formats from database views using SQL, pandas, plotly dash, and MikTex; outperformed a legacy Excel system by 100-fold
- Automated process of computing linear regressions on statewide educational metrics for over 500 school districts
- Designed and implemented a pipeline for estimating the probability a student will meet state education standards with calibrated support vector machines
- Created an interactive Dash website for visualizing and validating machine learning model performance on live educational data grouped by grade level and academic subject

Undergraduate Thesis Research / Computational Chemistry **SEP 2020 — APR 2021**
The Scholes Group *Princeton University, Princeton, NJ*
- Modeled catalyst empirical reaction efficiency as a function of simulation-obtained substrate binding free energies using GPU-accelerated molecular dynamics free energy calculations
- Computed visible spectrum of catalytic intermediate in agreement with experimental spectroscopy using Time Dependent Density Functional Theory
- Employed the weighted histogram analysis method to compute potentials of mean force from umbrella-sampled molecular dynamics trajectories

Summer Research Internship / Polymer Chemistry **JUN 2019 — AUG 2019**
The Lau Group *University of Strathclyde, Glasgow, UK*

- Modeled fluorescence time series data with Ward-Tordai equation for surface adsorption kinetics
- Implemented nonlinear regression and numerical integration algorithms for experimental data fitting to integro-differential equations
- Synthesized polymer nanosheets from peptide-like olgimers
- Developed and refined protocol to immobilize nanosheets on gold surfaces with thiol linkages for transmission electron microscopy

Publications

Unified Deep Learning Framework for Many-Body Quantum Chemistry via Green's Functions **AUG 2024**
Venturella, C.; Li, J.; Hillenbrand, C.; Peralta, X. L.; Liu, J.; Zhu, T. Unified Deep Learning Framework for Many-Body Quantum Chemistry via Green's Functions; 2024. arXiv:2407.20384

Machine learning many-body Green's function for molecular excitation spectra **OCT 2023**
C. Venturella, C. Hillenbrand, J. Li, and T. Zhu, "Machine Learning Many-Body Green's Functions for Molecular Excitation Spectra", J. Chem. Theory Comput. 2024, 20, 1, 143–154, arXiv:2310.09911

Modeling Nonnatural Flavoenzyme Catalysis with Molecular Dynamics and Quantum Chemical Methods **2021**
Princeton Undergraduate Thesis, Advisor(s): Gregory Scholes, Daniel Oblinsky

Presentations

American Chemical Society National Meeting, New Orleans (Abstract Link) **Spring 2024**
Presentation Title: Machine learning many-body Green's function for molecular excitation spectra

Teaching Experience

Teaching Fellow **SEP 2022 — Current**
Yale University Chemistry Department *New Haven, CT*

- General Chemistry I SEP 2022 — JUN 2023
- Physical Chemistry I (Thermodynamics and Kinetics) SEP 2023 — CURRENT

Undergraduate Teaching Assistant **SEP 2020 — MAY 2021**
Princeton University Chemistry Department *Princeton, NJ*

- Organic Chemistry I SEP 2020 — DEC 2020
- Organic Chemistry II JAN 2021 — MAY 2021

Trenton Arts Program Volunteer **SEP 2018 — MAY 2021**
Princeton University Music Department *Princeton, NJ*

- Private Music Instruction

Skills

Computational Chemistry
Python for chemical modeling and informatics (pyscf, geometric, ASE, rdkit), cp2k, Gaussian
Data Science and Data Engineering
Python for ML (scipy, sklearn, PyTorch, PyTorch Geometric, TensorFlow), python for data analytics and visualization (pandas, matplotlib, plotly, xlwings, dash, cvx, geopandas), SQL, MATLAB, R, Microsoft Excel
Mathematical Modeling
Kernel Ridge Regression, Gaussian Process Regression, Neural Networks, Geometric Deep Learning, Convex Optimization, Classifier Models, Model Calibration
Word Processing
LaTeX, HTML, Microsoft Word
Languages
English (Native), Spanish (Intermediate)