

Education

Yale University, New Haven, CT 08/2024-Present
Ph.D. Candidate in Theoretical Chemistry | Advisor: Prof. Victor Batista

Washington University in St. Louis, St. Louis, MO GPA: 3.99/4.00 08/2020-05/2024
A.B. Chemistry/Computer Science, Minor in Spanish | Summa Cum Laude

Experiences

Undergraduate Research Assistant, Washington University in St. Louis 08/2022-05/2024

- Contributed to research that led to a publication in JPC Letters titled "Two-Dimensional Infrared Spectroscopy of Isolated Molecular Ions."
- Assisted in writing data collection and processing algorithms.
- Developed a Dockerized environment for ORCA, ensuring scalable and reproducible computations.
- Collaborated closely with senior researchers, contributing to experiment maintenance and operation.

Assistant Instructor for Organic Chemistry Lab, Washington University in St. Louis 06/2022-05/2024

- Delivered experiment lectures and led 20-student lab sections.
- Collaborated with faculty and other instructors to optimize the curriculum and enhance student engagement and comprehension.

PACU Volunteer, Barnes Jewish Hospital 01/2023-01/2024

- Transported and escorted post-op patients, gaining familiarity with clinical protocols.
- Upheld strict sanitation standards post-patient departure.

Publications

Ma, Z., Chen, L., **Xu, C.**, & Fournier, J. A. (2023). Two-Dimensional Infrared Spectroscopy of Isolated Molecular Ions. *The Journal of Physical Chemistry Letters*, 14(43), 9683-9689.

Smaldone, A. M., Shee, Y., Kyro, G. W., **Xu, C.**, Vu, N. P., Dutta, R., ... & Batista, V. S. (2024). Quantum Machine Learning in Drug Discovery: Applications in Academia and Pharmaceutical Industries. *arXiv preprint arXiv:2409.15645*.

Dutta, R., Vu, N. P., **Xu, C.**, Lyu, N., Soudackov, A. V., Dan, X., ... & Batista, V. S. (2024). Simulating electronic structure on bosonic quantum computers. *arXiv preprint arXiv:2404.10222*.

Kyro, G. W., Smaldone, A. M., Shee, Y., **Xu, C.**, & Batista, V. S. (2024). T-ALPHA: A Hierarchical Transformer-Based Deep Neural Network for Protein-Ligand Binding Affinity Prediction With Uncertainty-Aware Self-Learning for Protein-Specific Alignment. *bioRxiv*, 2024-12.

Skills

Programming: Proficient in HTML, PHP, JavaScript, Python, C++, Swift, and Java. Experienced in packages including Tensorflow, PyTorch, Qiskit, PySCF, PyMOL, NumPy, Pandas,

Lab: Familiar with data processing and lab techniques from inorganic, physical, and organic chemistry labs.

Language: Fluent in Chinese and English. Proficient in Spanish.

Ski Instructor, Professional Ski Instructors of America: Led and mentored diverse groups, emphasizing effective communication of safety protocols and biomechanically-sound skiing techniques.