

# Anthony M. Smaldone

Theoretical Chemistry PhD Candidate at Yale University  
National Science Foundation Graduate Research Fellow  
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## SUMMARY

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I am a theoretical chemistry PhD candidate at Yale University and a National Science Foundation Graduate Research Fellow. As the Vice President and Co-Founder of Yale University's Biophysical Society and a key researcher in the QuantumCT NSF engine development initiative, I am committed to advancing interdisciplinary research at the intersection of quantum computing and machine learning.

My research focuses on developing quantum machine learning methods for pharmaceutical applications, leveraging both classical and quantum architectures to tackle complex molecular generation and drug discovery challenges. I have worked on a variety of projects, from designing quantum-enhanced transformers for molecular generation to introducing a novel quantum-classical convolutional neural network for toxicity prediction. I have published a quantum architecture in a high-impact journal that efficiently handles multi-channel data and achieved state-of-the-art performance among quantum neural networks on the CIFAR-10 dataset.

Beyond quantum machine learning, I am also interested in how classical machine learning can be leveraged to optimize quantum computing workflows. My ongoing projects explore the use of generative models and reinforcement learning to design efficient quantum circuits, with the goal of improving quantum algorithm performance for tasks such as state preparation and quantum chemistry. My expertise spans multiple quantum simulation frameworks, including CUDA-Q, PennyLane, and Cirq, and I have contributed to NVIDIA's CUDA Quantum documentation by developing a tutorial to help researchers implement quantum attention score calculations into their classical transformer workflows. This experience has deepened my understanding of GPU-accelerated quantum computing and its role in advancing real-world applications.

## EDUCATION

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<b>Yale University</b> <i>Doctorate of Philosophy in Theoretical Chemistry</i>	New Haven, CT, USA <i>05/2024 - Present</i>
<b>Yale University</b> <i>Master of Science in Theoretical Chemistry; GPA 4.00</i>	New Haven, CT, USA <i>08/2022 - 05/2024</i>
<b>State University of New York at Binghamton</b> <i>Bachelor of Science in Chemistry and Mathematics; GPA 3.96</i>	Binghamton, NY, USA <i>08/2019 - 05/2022</i>
<b>Corning Community College</b> <i>Associates of Science in Mathematics and Science; GPA 3.96</i>	Corning, NY, USA <i>08/2018 - 05/2019</i>

## PUBLICATIONS

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6. Pu, Y., Adrio, J., **Smaldone, A.M.**, Walsh, P., Sulfenate Anion Catalyzed Enantio- and Diastereoselective Aziridination (Submitted).
5. **Smaldone, A.M.**, Shee, Y., Kyro, G.W., Farag, M.H., Chandani, Z., Kyoseva, E., Batista, V.S., A Hybrid Transformer Architecture with a Quantized Self-Attention Mechanism Applied to Molecular Generation (Submitted). <https://arxiv.org/abs/2502.19214>.
4. Kyro, G.W., **Smaldone, A.M.**, Shee, Y., Chuzhi X., Batista, V.S., T-ALPHA: A Hierarchical Transformer-Based Deep Neural Network for Protein-Ligand Binding Affinity Prediction With

- Uncertainty-Aware Self-Learning for Protein-Specific Alignment. *ACS Journal of Chemical Information and Modeling* (2025). <https://pubs.acs.org/doi/10.1021/acs.jcim.4c02332>.
3. **Smaldone, A.M.**, Shee, Y., Kyro, G.W., Chuzhi, X., Vu, N.P., Dutta, R., Farag, M.H., Galda, A., Kumar, S., Kyoseva, E., Batista, V.S., Quantum Machine Learning in Drug Discovery: Applications in Academia and Pharmaceutical Industries. *ACS Chemical Reviews* (Accepted). <https://arxiv.org/abs/2409.15645>.
  2. **Smaldone, A.M.**, & Batista, V.S., Quantum to Classical Neural Network Transfer Learning Applied to Drug Toxicity Prediction (2024). <https://doi.org/10.1021/acs.jctc.4c00432>.
  1. **Smaldone, A.M.**, Kyro, G.W. & Batista, V.S., Quantum convolutional neural networks for multi-channel supervised learning. *Springer Nature Quantum Mach. Intell.* 5, 41 (2023). <https://doi.org/10.1007/s42484-023-00130-3>.

## POSTERS & PRESENTATIONS

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12. Quantum Machine Learning Methods for Drug Safety Prediction. Invited research talk at *QuantumCT Industry Collaboration Forum, Yale Ventures, 2025*.
11. A Hybrid Transformer Architecture with a Quantized Self-Attention Mechanism Applied to Molecular Generation. *AI4Quantum Conference, Novo Nordisk Foundation Science Cluster, Denmark, 2025*. Poster Prize Winner.
10. T-ALPHA: A Hierarchical Transformer-Based Deep Neural Network for Protein-Ligand Binding Affinity Prediction With Uncertainty-Aware Self-Learning for Protein-Specific Alignment. Poster Presentation at Chemical Research Symposium at *Yale University, 2025*.
9. Leveraging Quantum Circuits for Generative Chemistry. Poster Presentation at Chemical Research Symposium at *Yale University, 2025*.
8. Hybrid Quantum-Classical Neural Networks for Drug Discovery. Invited research talk at *Quantum IEEE 2024, Quantum for Bio and Life Sciences Workshop, 2024*.
7. Accelerating Drug Design with Quantum Computation. Invited research talk at the *Computational Biophysics and Drug Design Meeting, Bernal Institute at the University of Limerick, 2024*.
6. Quantum to Classical Neural Network Transfer Learning Applied to Drug Toxicity Prediction. *CCG & UGM and Conference, North America 2024*.
5. Hybrid Classical-Quantum Neural Networks for Drug Discovery. Invited research talk at *QuantumCT Industry Collaboration Forum, Yale West Campus, 2024*.
4. The Integration of Machine Learning and Quantum Computing. Invited guest lecture at *CHEM 584: Machine Learning and Quantum Computing, Yale University, 2024*.
3. Understanding the Sulfite Sensing Ability of 4-(1H-pyrrol-2-yl) pyridine with Density Functional Theory. *Binghamton ACS Poster Session, 2022*.
2. Sulfenate Anion-Catalyzed Enantioselective Aziridination. *University of Pennsylvania NSF REU Presentation Session, 2021*.
1. Density Functional Theory Analysis of Ni-Doped MnO<sub>2</sub> in Multivalent Ion Battery Applications. *Binghamton Research Days Poster Session, 2020*.

## TECHNOLOGICAL SKILLS

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**Languages/Scripts:** Python, Java, Bash, HTML, Batch

**Programs/Systems:** PyTorch, Tensorflow, Scikit-Learn, Pennylane, Qiskit, Cuda Quantum, Cirq, RDKit, Gaussian Suite, Unix, Latex, FAISS, NERSC, Synology NAS

**Methods:** Deep Learning, Transformers, Reinforcement Learning, CNNs, GNNs, GANs, K-Means, Spherical K-Means, PCA, Variational Quantum Circuits, Quantum Machine Learning, Quantum Algorithms, Quantum Computational Chemistry

## RESEARCH EXPERIENCE

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### Graduate Research Experience

*Batista Lab*

01/2023 – Present  
New Haven, CT, USA

- Developing methods to combine machine learning and quantum computing
- Developed novel quantum self-attention algorithm for use in a transformer
- Published state-of-the-art quantum convolutional neural network in a high-impact journal
- Developed the first quantum-to-classical transfer learning framework for weight fine-tuning
- Fostered collaborations between Pfizer, Moderna, Yale, and University of Connecticut faculty through the QuantumCT initiative
- Collaborated with NVIDIA on CUDA-Q, contributing a tutorial on quantum attention score calculations in classical transformer workflows

### Undergraduate Research Assistant

*Lees Lab*

06/2020 – 06/2022  
Binghamton, NY, USA

- Performed DFT, TDDFT using Gaussian Suite on chemical sensors
- Organic synthesis of sulfite sensors
- Characterizations with NMR and UV-Vis

### NSF REU Research Assistant

*Walsh Lab*

05/2021 – 08/2021  
Philadelphia, PA, USA

- Synthesized a range of asymmetric organocatalysts
- Flash and column chromatography

### Summer Immersion Research Assistant

*Smeu Lab*

05/2020 – 08/2020  
Binghamton, NY, USA

- DFT calculations of periodic systems using Quantum Espresso
- Search for energy storage alternatives using multi-valent ion batteries

## RELEVANT COURSEWORK

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### • Chemistry and Physics Coursework

- \* Analytical Chemistry
- \* Calculus-based Physics I
- \* Calculus-based Physics II
- \* Computational Chemistry
- \* Experimental Physical Chemistry
- \* Intermediate Inorganic Chemistry
- \* Instrumental Methods and Analysis
- \* Introduction to Quantum Mechanics I
- \* Introduction to Quantum Mechanics II
- \* Introduction to Statistical Mechanics I
- \* Introduction to Statistical Mechanics II
- \* Molecular Photochemistry
- \* Molecules and Radiation: Matrix Methods in Quantum Mechanics I
- \* Molecules and Radiation: Matrix Methods in Quantum Mechanics II
- \* Physical Chemistry
- \* Physical Inorganic Chemistry
- \* Physical Organic Chemistry
- \* Quantum Chemistry and Spectroscopy
- \* Research in Smart Energy I
- \* Research in Smart Energy II

- \* Organic Chemistry I
- \* Organic Chemistry II
- \* Organic Chemistry Laboratory
- Mathematics and Computer Science Coursework
  - \* Advanced Linear Algebra
  - \* Applied Machine Learning
  - \* Computer Science and the Modern Intellectual Agenda
  - \* Differential Equations (Proof based)
  - \* Dynamical Systems
  - \* Foundations of Geometry
  - \* Linear Algebra
  - \* Machine Learning and Quantum Computing
  - \* Multivariable Calculus
  - \* Number Systems
  - \* Partial Differential Equations
  - \* Topics in the History of Mathematics

## LEADERSHIP, VOLUNTEER, EXTRACURRICULAR

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- Co-Founder & Vice President of the Yale University Student Chapter of the Biophysical Society Feb 2024 – Present
  - Manage funding and expenditures of the society
  - Coordinate debate events hosted by the Biophysical Society
- Co-Founder of Illuminating Minds Academy 10/2023 – Present
  - Offers personalized tutoring sessions in a multitude of STEM subjects
  - Strategic college preparation
  - Essay writing, coding tutorials, CV development
- Graduate Student Mentor 06/2023 – 08/2023
  - Mentored two first-year graduate students, facilitating a smooth transition and fostering a welcoming environment
  - Conducted meetings, addressing concerns, providing information, and promoting open communication to enhance the comfort and confidence of first-year graduate students in the department
- Founder of STEM Youth Outreach Program 07/2021 – 04/2024
  - A volunteer organization aimed to expose pre-adolescents in Title 1 classified school districts to STEM
  - 300 students reached
- Undergraduate Chemistry Mentor 08/2021 – 05/2022
  - Mentor in the Smart Energy Scholars Mentor Program
  - Mentor in the Binghamton University Chemistry Club
- Student Association Executive Board Treasurer at Corning Community College 08/2018 – 05/2019
  - Acted as Budget Committee Chairman
  - Created/passed budget of funds exceeding \$280,000 for the 2019-2020 academic year
  - Managed Executive Board Funds exceeding \$40,000 with zero deficiencies
  - Developed criteria to approve the dispensing of funds to clubs and organizations
- Debate Club Founder and President at Corning Community College 08/2018 – 05/2019
  - Secured collegiate funding for club expenses
  - Held formal and informal debates
  - Instructed members on refining their debate skills

## WORK AND TEACHING EXPERIENCE

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- Trainer for Large Language Models - Coding & Mathematics 01/2024 – 05/2024
  - Corrected outputs from large language models to correctly solve coding and math problems
  - Design difficult math and physics problems to stump LLMs
  - Developed unit tests to evaluate the accuracy and reliability of LLMs in solving coding problems
- Graduate Teaching Assistant for General Chemistry I 08/2022 – 05/2023
  - Aided Professor Nilay Hazari and Professor Paul Cooper in grading and exam proctoring
  - Administered two weekly one hour discussions
  - Held weekly office hour
- Undergraduate Teaching Assistant for Inorganic Chemistry 08/2020 – 12/2020
  - Administered weekly two hour discussions
  - Held weekly office hours
- Network Technician at Corning-Painted Post School District Summers of 2018 and 2019
  - Built computer labs
  - Mass updated laptops' BIOS and software

## HONORS AND AWARDS

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- NSF Graduate Research Fellowship (\$147,000)
- NIH Biophysical Training Grant (\$27,000)
- AI4Quantum Poster Prize Winner
- Yale Teaching Fellowship
- NSF Graduate Research Fellowship Honorable Mention
- American Chemical Society Outstanding Senior Award
- Smart Energy Scholarship (\$30,000)
- CCC Presidential Scholarship (\$5,600)
- Evans Roofing Company Inc. Scholarship (\$4,400)
- Summer Research Immersion Scholarship (\$2,400)
- Dr. Nathan V. Cooper Memorial Scholarship (\$1,400)
- Binghamton University Dean's List
- Corning Community College President's List
- Phi Beta Kappa Honors Society
- Phi Theta Kappa Honor Society
- Tau Sigma Honors Society
- Pi Mu Epsilon Honor Society