SAMUEL SCOTT TAYLOR

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EDUCATION

University of Chicago | Chicago, IL **September 2025 - Present**
Ph.D. | Quantum Science and Engineering
NSF GRFP Fellow & PME Graduate Fellow
Advisor: Giulia Galli

Vanderbilt University | Nashville, TN **August 2021 - May 2025**
Bachelor of Science | Physics (Highest Honors), Computer Science, Applied Mathematics (Triple Major)
Minor: Scientific Computing
Thesis: "Fragmentation in Coulomb Explosion of Hydrocarbons"
Advisor: Kálmán Varga

RESEARCH INTERESTS

- Computational nanoscience and materials
- Non-adiabatic dynamics of excited states
- Light–matter interactions
- Quantum materials and solid-state spin defects
- Electronic-structure theory (DFT / TDDFT)
- Numerical algorithms for large-scale simulations
- Many-body and excited-state phenomena
- Machine learning for materials modeling

PUBLICATIONS

View my Google Scholar profile

Misa Viveiros, **Samuel S. Taylor**, Cody Covington, Kálmán Varga. (2025) "*Ab initio* study of highly charged ion–induced Coulomb explosion imaging", *Physical Review A* (under review). https://doi.org/10.48550/arXiv.2512.08102

Misa Viveiros, Roy Lau, **Samuel S. Taylor**, Patrick Barron, Attila Czirjak, Cody Covington, Kálmán Varga. (2025) "Low-energy proton impact dynamics on hydrocarbons: Dependence on kinetic energy and incident site", *The Journal of Chemical Physics* (under review). https://doi.org/10.48550/arXiv.2509.16252

C. Jiang, **Samuel S. Taylor**, Kedong Wang, Cody L. Covington, Kálmán Varga. (2025). "Time-dependent density functional theory investigation of the formation of H^{3+} from alkanes", *The Journal of Chemical Physics* **163**(21), 214101. https://doi.org/10.1063/5.0296066

Samuel S. Taylor, Nicholas Skoufis, Hongbo Du, Cody Covington, Kálmán Varga. (2025). "Hydrogen adsorption and scattering on graphene with electron dynamics: Effects of incident point and kinetic energy", *Physical Review A* **112**, 032812. https://doi.org/10.1103/zkwl-sj59

Karoly Mogyorosi, Balint Toth, Krisztina Sarosi, Barnabas Gilicze, Janos Csontos, Tamas Somoskoi, Szabolcs Toth, Prabhash Prasannan Geetha, Laszlo Toth, **Samuel S. Taylor**, Nicholas Skoufis, Liam Barron, Kalman Varga, Cody Covington, Viktor Chikan. (2025). "CH(A) Radical Formation in Coulomb Explosion from Butane Seeded Plasma Generated with Chirp-Controlled Ultrashort Laser Pulses", *ACS Omega* **10**, 25285. https://doi.org/10.1021/acsomega.4c11074

Samuel S. Taylor, Cody Covington, Kálmán Varga. (2025). "Quantum effects of Coulomb explosion simulations revealed by time-dependent density-functional theory", *Physical Review A* **111**, 033109. https://doi.org/10.1103/PhysRevA.111.033109

Samuel S. Taylor, Robert J. Scherrer. (2025). "What do we learn by mapping dark energy to a single value of w?", *Physical Review D* **111**, 043534. https://doi.org/10.1103/PhysRevD.111.043534

Samuel S. Taylor, Kálmán Varga, Károly Mogyorósi, Viktor Chikán, Cody Covington. (2025). "Fragmentation in Coulomb explosion of hydrocarbon molecules", *Physical Review A* **111**, 013109. https://doi.org/10.1103/PhysRevA.111.013109

SKILLS

Python, C++, Fortran, Bash, Make, OpenMP, CUDA, PyTorch, TensorFlow, SSH, Blender, Quantum Espresso, WEST, SALMON, XCrySDen, VisIt, Mathematica, React, LaTeX

RESEARCH EXPERIENCES

Pritzker School of Molecular Engineering at UChicago | Chicago, IL **September 2025 – Present**
Ph.D. Student Researcher
PI: Dr. Giulia Galli

- Development of non-adiabatic molecular dynamics using **linear-response TDDFT**
- First-principles implementation of surface-hopping excited-state dynamics in **WEST**

Vanderbilt University | Nashville, TN **August 2023 - August 2025**
Research Assistant: Computational Nanoscience
PI: Dr. Kálmán Varga

- Generated over **2 TB** of light-matter interactions, molecular collisions, and graphene hydrogenation simulation data on the Texas A&M ACES supercomputer and the research group's remote **Linux** cluster
- Developed more than **20,000** lines of **Fortran90**, **Make**, **Bash**, **C++**, and **Python** code across projects, including simulations and visualizations for classical Coulomb explosions and implementing Boltzmann-distributed molecular velocities to enhance real-time TDDFT capabilities
- Directly mentored over **15 students** on TDDFT, simulation setup and execution, and result analysis, including creating hours of instructional YouTube tutorials for the research group

ELI-ALPS Laser Research Institute | Szeged, Hungary **May 2024 / 2025 - August 2024 / 2025**
Research Assistant: Ultrafast Dynamics Group / Theory and Simulation Group
PI: Dr. Károly Mogyorósi / Dr. Attila Czirják

- Executed more than **350 real-time TDDFT simulations** on Coulomb explosion of the first four alkanes, utilizing experimental pulse input data to predict fragmentation patterns;
- Computed the polarization potential in high-harmonic generation (HHG) of argon, incorporating it as a correction to improve the single-active-electron approximation
- Delivered an **hour-long presentation** to **25 attendees**, including research group leaders at ELI-ALPS and professors from the University of Szeged. Explained TDDFT principles and its application to ELI-ALPS experiments, initiating an ongoing collaboration between ELI-ALPS and Vanderbilt University

Vanderbilt University | Nashville, TN **January 2025 - May 2025**
Research Assistant: Computer Graphics, Numerical Methods, and Machine Learning
PI: Dr. David Hyde

- Designed and implemented a deep learning based convolutional neural network (**CNN**) to enhance the **MINRES**, **GMRES**, and **BiCGSTAB** algorithms for solving linear systems, replacing traditional iterative search direction calculations with **ML** predictions to significantly improve computational efficiency
- Numerically solved the incompressible Euler equations and rendered results in **Houdini** and **Blender**

University of Tsukuba | Tsukuba, Ibaraki, Japan **May 2023 - July 2023**
Research Assistant
PI: Dr. Kazuhiro Yabana

- Performed density-functional theory **(DFT)** calculations using **SALMON** (Scalable Ab-initio Light-Matter Simulator for Optics and Nanoscience) software with the jellium model for constructing metamaterial simulations
- Conducted quantum electrodynamic DFT **(QED-DFT)** simulations to investigate energy shifts and electronic structure differences between left- and right-handed enantiomers of H_4 and H_2O_2 molecules within chiral cavities exposed to circularly polarized light fields
- Visualized intricate simulation results and presented findings in weekly meetings, utilizing **Python**, **JMol**, and **VisIt** to effectively communicate insights to the research team

Vanderbilt University | Nashville, TN **February 2022 - May 2023**
Research Assistant: Cosmology
PI: Dr. Robert Scherrer

- Conducted independent research under Dr. Robert Scherrer, focusing on mapping various dark energy equation of state parametrizations, including Chevallier-Polarski-Linder and Hilltop models (with $K = 2$ to $K = 4$), to constant w. Determined and visualized the best-fit w and the redshift pivot for various w_0 and w_a inputs
- Developed over 1,000 lines of Python code using **NumPy**, **SciPy**, and **Matplotlib** to compute luminosity distances, redshift, and chi-squared error, and to create figures for visualizing and analyzing dark energy models

RELEVANT COURSEWORK

Advanced Quantum Engineering, Graduate Quantum Mechanics, Machine Learning, Partial Differential Equations, Numerical Mathematics, Computer Simulation, Quantum Mechanics I & II, Software Engineering, Algorithms

AWARDS/HONORS

- NSF GRFP (2025-2030)
- Vanderbilt Highest Honors in Physics (2025)
- Underwood Memorial award (2025)
- Alex Taylor Education Enhancement Fund (2025)
- Dean's list (all semesters, 2021 – 2025)
- PME Graduate Fellowship (2025)
- Yaquiong Xu Best Publication award (2025)
- Sigma Pi Sigma (2024)
- Pi Mu Epsilon (2025)
- Tau Beta Pi (2025)

ACTIVITIES AND LEADERSHIP

Society of Physics Students | Nashville, TN **August 2024 - May 2025**
Social Chair

- Organized social events, guest lectures, networking opportunities, increasing student engagement and turnout by **30%**
- Presented research and delivered presentations to give students opportunities to engage in research, increasing the size of Dr. Varga's computational nanoscience research group by over **20%**

Blair Big Band | Nashville, TN **August 2021 - May 2024**
Jazz Saxophonist

- Achieved finalist status in the 2023 Jack Rudin Jazz Championship at Jazz at Lincoln Center in New York City, ranking among the top four ensembles nationwide
- Studied jazz saxophone under three-time Grammy-winning saxophonist and Rock & Roll Hall of Fame inductee Jeff Coffin (Dave Matthews Band)

REFERENCES

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