Jared Keith Averitt

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EDUCATION

University of North Carolina Greensboro — Greensboro, NC
- National Science Foundation Graduate Research Fellow (2021318933) — 2020 — 2024
- Ph.D., Nanoscience and Material Science (3.96 GPA)
- Dissertation: *Modeling the Dynamics of 2D Nanoscale Devices: From Classical Physics to Quantum Theory and Machine Learning Perspectives* — Conferral, May 2nd, 2024
  - Committee Chairs: Dr. Tetyana Ignatova and Dr. Joseph Starobin
- Additional Graduate Physics Coursework at Duke University

Austin Peay State University — Clarksville, TN
- B.S., Physics Major - Mathematics Minor (3.93 GPA) — 2018 — 2020
- B.S., Biology Major - Chemistry Minor (3.38 GPA) — 2010 — 2020
- Additional Coursework at Middle Tennessee State University

PROFICIENT COMPUTATIONAL RESEARCH SKILLS

- Density Functional Theory (VASP, Gaussian16)
- Machine Learning (TorchANI, PyTorch, Scikit-learn)
- High Performance Computing and programming (openMPI, CUDA, GPU)
- Finite Element Modeling (COMSOL Multiphysics)
- Programing Languages (Fortran, C++, Python, MATLAB, Mathematica)
- Atomic and Molecular Tools (PyMol, VMD, Chemcraft, ASE, Multiwfn)
- LaTeX, PGFPlots, TikZ
- Molecular Dynamics (ReaxFF, SDF)
- Mac OS, Linux and Windows

PUBLICATIONS

[1] **Jared Averitt,** Sajedeh Pourianejad, Olubunmi O Ayodelle, Anthony Trofe, Kirby Schmidt, Joeseph Starobin, Tetyana Ignatova, "Efficient High-Throughput Method Utilizing Potential Neural Networks, Validated by Clean Transfer Experiment of CVD Graphene with Polymer Mixtures". arXiv. 2023 October. https://arxiv.org/abs/2310.10020 DOI: 10.48550/ARXIV.2310.10020 (in review in *Carbon*)

[2] **Jared Averitt**, Anthony Trofe, Sajedeh Pourianejad, Tetyana Ignatova, "Shielding effect of water in Kelvin Probe Force Microscopy: experimental and finite element analysis approach", 2024, In preparation (expected submission to *IEEE* March 2024)

[3] **Jared Averitt**, Wesley Reinhart, Vincent Crespi, Joeseph Starobin, Tetyana Ignatova, "Neural Network method for the discovery of nanoscale optical-based sensors of ammonia and phosphate compounds", 2024, In preparation (expected submission in April 2024)

[4] Olubunmi O Ayodelle , Adeyinka O Adesina, Sajedeh Pourianejad, **Jared Averitt** , Tetyana Ignatova, "Recent Advances in Nanomaterial-Based Aptasensors in Medical Diagnosis and Therapy" Nanomaterials (Basel), April, 2021 6;11(4):932. https://www.mdpi.com/2079-4991/11/4/932

[5] S. Markov, **J. Averitt**, B. Waldron. "Bioreactor for glycerol conversion into H_2 by bacterium Enterobacter aerogenes" International Journal of Hydrogen Energy, January 2001 Vol 36, 2011. P 262-266. https://linkinghub.elsevier.com/retrieve/pii/S0360319910020008

CONFERENCE PRESENTATIONS

[1] **J.K. Averitt,** Joeseph Starobin, Tetyana Ignatova. "Deconvolution the Electric-Shielding Effect of Ubiquitous Water in Kelvin Probe Force Microscopy: Finite Element Approach". American Physical Society, March Meeting. Virtual, March 3-8, 2024.

[2] Besan Khader, Pearson Hart, Arif Khan, **Jared Averitt**, Aleksandrs Prokofjevs, Tetyana Ignatova. "Development of Nanoscale Optical Sensor for Ammonia Detection". American Physical Society, March Meeting. Virtual, March 3-8, 2024.

[3] **J.K. Averitt**, Joeseph Starobin, Tetyana Ignatova. "Computational Materials Design of Optical Based Nanoscale Sensing Devices". NSF Nanoscale Science and Engineering Grantees Conference. Alexandria, VA. December 7-8, 2023. Poster https://www.nseresearch.org/2023/posters/Jared_Averitt_NSF_Grantees_Poster_11_2023.pdf

[4] **J.K. Averitt,** Joeseph Starobin, Tetyana Ignatova. "High throughput Potential Neural Network Method to exploit non-local interactions on graphene interface". 2DLM/2DCC Graphene and Beyond Workshop. University Park, PA. May 17-18, 2023. Poster

[5] **J.K. Averitt,** Sajedeh Pourianejad, Olubunmi Ayodelle, Tetyana Ignatova. "Electronic structure simulations of polymer(s) on graphene through a potential neural network". American Physical Society, March Meeting. Virtual, March 20-22, 2023. Poster

[6] **Jared Averitt**, Anthony Trofe, Joseph Starobin, Tetyana Ignatova, Micheal Ghebrebrham."Development of Maximal Scattering Camouflage Clothing for Soldiers Using 2D Materials", Grand opening of ICONS ,Greensboro NC. November 21, 2022. Poster

[7] **Jared K. Averitt**, Besan Khader, Joseph Starobin, Tetyana Ignatova, Micheal Ghebrebrham."Screening Library of in-silico Pyrene-graphene Based Sensors", Grand opening of ICONS, Greensboro NC. November 21, 2022. Poster

[8] S. Kalkar, A. Adesina, **J. Averitt**, D. Herr, T. Ignatova. "Tailoring Properties of Cyanobacteria with SWCNT Hybrid". NanoImpacts 2022: SemiSynBio and Beyond, Greensboro NC. October 13 -15, 2022.

[9] **J.K. Averitt,** Sajedeh Pourianejad, Olubunmi Ayodelle, Tetyana Ignatova. "Energy decomposition analysis from DFT investigations of polymer(s) on graphene". 2DLM/2DCC Graphene and Beyond Workshop. University Park, PA. May 18-19, 2022. Poster

[10] **J.K. Averitt,** Sajedeh Pourianejad, Olubunmi Ayodelle, Tetyana Ignatova. "DFT simulation of polymer(s) on graphene: Polymer confirmation and adhesion energy considerations". American Physical Society, March Meeting. Chicago, IL. March 14-18, 2022. Poster

[11] Sajedeh Pourianejad, **J. Averitt**, O. Ayanbajo, S. Aravamudhan, T. Ignatova, "Work function modulation in 2D MoS_2". Carolina Science Symposium. Virtual, November 12-13, 2020. Poster

[12] **J. Averitt**, M. Mouton, K. Webster, J. Shajahan, A. Maselugbo, S. Loeffler. "Summary of the UN GCO-II", Virtual networking session entitled: "Convergence Research for the Biorefinery: A Networking Session". June 22, 2020. Oral

[13] **J.K. Averitt**, R. Golovchak. "Positron Annihilation Lifetime Spectroscopy of Natural Quartz (SiO_2)". NASA Southeast Regional Space Grant Meeting. Nashville, TN. September 26-27, 2019. Poster

[14] **J.K. Averitt**, R. Golovchak. "Re-usable $\beta+$ source - sample sandwich for positron annihilation lifetime spectroscopy". Annual Meeting of the Tennessee Section of the American Association of Physics Teachers. (TAAPT 2019). Knoxville, TN. March 29-30, 2019. Poster

CONFERENCE PRESENTATIONS (CONTINUED)

[15] **J.K. Averitt**, R. Golovchak. "Re-usable Positron Source for Non-Destructive Positron Annihilation Lifetime Spectroscopy of Solids". Tennessee Posters at the Capitol. Nashville, TN. Feburary 26, 2019.

[16] **J. Averitt**, S. Markov. "Hydrogen Production from Malate or Glycerol by Purple Non-Sulfur Photosynthetic Bacteria". Bioenergy Sustainability Conference. Nashville, TN, October 21-23, 2019.

[17] **J.K. Averitt**, R. Golovchak. "Design and Preparation of Positron Source for Non-Destructive Positron Annihilation Lifetime Spectroscopy". 85th Annual Meeting of the APS Southeastern Section (SESAPS-2018). Knoxville, TN, Nov. 8–10, 2018. *Bulletin of the American Physical Society*. Abstract: D05.00042. Poster

[18] **J. Averitt**, S. Childs, S. Markov. "Biomass and oil production by microalga *Neochloris oleoabundans* in floating, rocking and stationary bag photobioreactors". National Conference on Undergraduate Research (NCUR-2018). Oklahoma City, OK. April 4-7, 2018. Poster

[19] **J.K. Averitt**, S. Markov. "Novel floating-type photobioreactor for microalga growth and biofuel production". 125th Annual Meeting of Tennessee Academy of Science (TAS-2015), Murfreesboro, TN. November 20, 2015. Oral

[20] **J. Averitt**, S. Markov. "Bioreactor for glycerol conversion into H_2 and ethanol by bacterium Enterobacter aerogenes" 111th Annual General Meeting of American Society for Microbiology (ASM-2011). New Orleans, LA. May 21-24, 2011. Poster

HONORS, AWARDS, FELLOWSHIPS, GRANTS AND SCHOLARSHIPS

- NSF Graduate Research Fellowship Program (no. 1945980, ID: 2021318933) $155,000   2021 – 2024

- NSF XSEDE Start-up Allocations (PHY220034) : Modeling of molecules adsorbed on the surface of 2D materials: multi-component analysis $516   2022 – 2023

- Educational Peltier Cooler for Teaching and Research Advancements (004645) : UNCG Graduate Student Association Research Capstone Fund $294.35   November 2023

- Humidity Sensor / Controller for Atmospheric Atomic Force Microscopy (003196) : UNCG Graduate Student Association Research Capstone Fund $299.35   Feburary 2022

- Study of fundamental properties of two-dimensional platform for biosensor application (001775) : UNCG Graduate Student Association Research Capstone Fund $300   October 2020

- Dean's List : APSU   2017 – 2020

- NASA Scholarship : Tennessee Space Grant Consortium (no. NNX15AR73H) $6,000   2018 – 2019

- Summer Undergraduate Research Fellowship : APSU $5,000   2018 – 2019

- Presidential Research Scholarship "H2 Production from Malate or Glycerol by Photosynthetic Bacteria" : APSU $2,000   2016 – 2017

GRADUATE RESEARCH EXPERIENCE

The Pennsylvania State University State College, PA
Visiting Research Scholar with Dr. Vincent Crespi, Dr. Adri van Duin, Dr. Weiss Reinhart May 2023 – present

- I have engaged in computational research within the NSF-funded Two-Dimensional Crystal Consortium – Materials Innovation Platform Theory Group, focusing on the development of a neural network and algorithm tailored for the design of MoS2-Pyrene optical sensors. Our work includes conducting reactive force-field (ReaxFF) simulations to understand the behavior of polymer adhesion on defective graphene surfaces. This research has been disseminated through three poster presentations, and we are in the process of preparing a manuscript based on these findings.

US Department of Defense Army DEVCOM Soldier Center Natick, MA
Graduate Student Scholar in Partnership with The Joint School Of Nanoscience and Nanoengineering (#W911QY2220006) 2022 - present

- Engaging with soldiers and veterans, I led the project modeling the electronic structure modulation of 2D material based sensors for their ability to detect ammonia and phosphate compounds using. This resulted in an effort I led, to create a graph convolutional network for predicting fermi-energy shifts given a composition of molecules adsorbed on graphene I've shared these findings through three posters. This work focuses on creating sensors suitable for extreme environments to enhance soldier safety.Effective simulated sensors depended on significant changes in their band structures, as these alterations were expected to impact fluorescence and Raman signals.

Nano-Opto-Bio Lab, University of North Carolina at Greensboro Greensboro, NC
NSF Graduate Research Fellow (no. 1945980, ID: 2021318933) 2020 - present

- I have spearheaded the development of computational techniques for nano-scale analysis, incorporating Neural Networks and Density Functional Theory (DFT). We focused on the optimization of solid-state optoelectronic sensor designs and the quantification of polymer adhesion energies critical for graphene transfer methods. Moreover, I led the investigation on the effects of water's electrostatic potential shielding in various environments employing the Finite Element Method (FEM). This work includes authoring or co-authoring several papers and presenting our findings in six poster presentations, with one paper currently under peer review and another in the stages of submission.

MEMBERSHIP OF PROFESSIONAL SOCIETIES

Materials Research Society : JSNN Student Chapter	2021 – present
American Physical Society	2018 – present
Sigma Phi Sigma Physics Honor Society	2018 – present
Del Square Psi : APSU Student Chapter of Sigma Phi Sigma	2018 – 2020
Tri-Beta Biological Honor Society	2010 – 2020

SYNERGISTIC ACTIVITIES

- **Instructor, AI Methods in Advanced Materials Research** : Designing and executing a course in January - May 2024 at the Joint School of Nanoscience and Nanoengineering in Greensboro, NC, for equipping graduate students with essential Machine Learning and Neural Network skills tailored for materials research, encompassing convolutional neural networks, Bayesian analysis, and advanced techniques. Course Website : https://github.com/JaredKeithAveritt/AI_methods_in_advanced_materials_research

- **K-12 Physicist To-Go Volunteer with the American Physical Society:** Engaging in a remote capacity since 2020, virtually connecting with twelve demographically diverse classrooms spanning multiple states such as PA, CO, TX, TN, NC, and MA. Facilitating interactive sessions by fielding inquiries from K-12 students about the role of physicists while fostering enthusiasm for physics, aiming to inspire the next generation to delve into scientific exploration.

- **K-5 North Central Region 5 Science and Engineering Fair Mathematics and Physics Judge:** Since 2021, I have been providing constructive feedback on student projects and offering guidance to emerging scientists and engineers. My goal is to acknowledge and affirm their endeavors in advancing scientific knowledge, fostering an environment of growth and learning.

- **Ad hoc Reviewer for the Southeastern Section of the American Physical Society**: I participated in the evaluation and selection process for the prestigious annual Jesse W. Beams Award, contributing to the recognition of outstanding research achievements.

- **K-12 Outreach Events Volunteer** : Since 2021, I have been actively contributing to The Joint School of Nanoscience and Nanoengineering in Greensboro, NC, where I participated in a team of graduate students to deliver hands-on demonstrations in Nanoscience to spark enthusiasm for STEM education among students. Additionally, I serve as a Graduate Researcher Panelist, providing valuable insights and guidance to undergraduates interested in pursuing a Ph.D. in materials science.

- **Mentor, Draelos Scholar Program** :I led a ten-week research project, teaching two students about machine learning, High Performance Computing, and Density Functional Theory. They applied these skills to study nanoscale devices, culminating in five-minute presentations at the program's end.

- **Graduate Student Peer Mentor, The Joint School of Nanoscience and Nanoengineering :** Since 2021, I've mentored seven STEM-track graduate students with four combined publications, from countries including Ghana, Bangladesh, and Jordan. I conduct weekly sessions for three junior lab members on topics such as grant writing, research techniques, publishing, and professional development.

- **Education Outreach Volunteer in Nalerigu, Ghana**: during June to July 2010, I collaborated with the Baptist Medical Center and a remote village impacted by tuberculosis. By fostering cultural harmony and building strong connections, I significantly contributed to the success of education initiatives and the effective distribution of vaccinations.

NON-COMPUTATIONAL RESEARCH SKILLS

Biochemical Analysis
- PCR (Quantitative, Real-time)
- ELISA
- Horizontal gene transformations

Microscopy
- Confocal (bright field, phase contrast)
- Wide Field Fluorescence
- Differential interference contrast (DIC)

Materials Characterization
- Positron Annihilation Lifetime Spectroscopy (ORTEC)
- Confocal Raman Spectroscopy (HORIBA XploRA)
- SEM (Hitachi S-3400, Oxford Aztec INCA X-Act)

Chemical Analysis
- NMR (Bruker Fourier 300)
- UV-Vis (HP 8453)
- FTIR (Bruker Tensor 27)

UNDERGRADUATE RESEARCH EXPERIENCE

Materials Fabrication and Characterization Lab, Austin Peay State University
Undergraduate Research Assistant with Dr. Roman Holovchak and Dr. Andriy Kovalskiy

Clarksville, TN
2018 - 2020

- Collaborated with the Physics and Geology departments to use Positron Annihilation Lifetime Spectroscopy (PALS) for analyzing water inclusions in quartz. Developed a device for precise radioactive positron deposition on thin films and a 3D-printed tool for accurate source positioning. Analyzed PALS data and presented findings in three posters.

Microorganism based Biofuel Production Lab, Austin Peay State University
Undergraduate Research Assistant with Dr. Sergei Markov

Clarksville, TN
2009 - 2012

and
2016 - 2018

- Supervised and trained three researchers, fine-tuned bioreactor conditions for enhanced biofuel production, performed chemical analyses for data collection, co-authored a peer-reviewed article, and presented four posters and one oral presentation.

LEADERSHIP, MENTORING AND TEACHING EXPERIENCE

Govenor's School for Computational Physics
Teaching Assistant and Resident Mentor with Dr. Alex King and Dr. Daniel Mayo

Clarksville, TN
2019 - 2020

- Managed grading, led experiments, and offered individual support and mentoring for 41 high school students enrolled in a Computational Physics Method course. This was part of an intensive three-week, seven-college-credit pre-college STEM program, conducted across two separate cohorts.

Tri-County (TRIO) Upward Bound, Austin Peay State University
Instructor for Mathematics and Physics with Upward Bound director, Melissa Conwell

Clarksville, TN
2019 - 2020

- Designed and implemented engaging lesson plans for a 5-week Department of Education-funded pre-college preparatory program aimed at economically disadvantaged high school students, while maintaining academic records.
- Coordinated with the APSU Physics Department's lab manager to secure the same resources for our program as those provided to Gov School students, ensuring TRIO participants have access to these resources for future cohorts.

Physics Department, Austin Peay State University
Teaching Assistant for undergraduates

Clarksville, TN
2018 - 2020

- Led bi-weekly recitations and worked closely with faculty to strengthen student-professor relationships, facilitating discussions to identify learning gaps. This experience exposed me to diverse teaching methods and enhanced my understanding of student learning needs, helping them grasp course material and succeed academically.

- Supported courses and instructors include:
    - Calculus-based Physics (Dr. Roman Holovchak and Dr. William Longhurst)
    - Algebra-based Physics (Dr. Xiong Pei, Dr. Andriy Kovalskiy, and Dr. Arthur Carpenter)

LEADERSHIP, MENTORING AND TEACHING EXPERIENCE (CONTINUED)

Mathematics Department, Austin Peay State University   Clarksville, TN
Teaching Assistant for undergraduates   2018 - 2020

- Empowered students with deficiencies in mathematics to rethink their study habits and to improve their mathematics skills. Developed specific lesson plans for the students to reinforce the concepts they were learning in class while also improving their skills in algebra.
- Supported courses (Instructors):
  - ▸ Single-variable Calculus (Dr. Daniel Mayo)
  - ▸ Elementary Statistics (Dr. Ben Ntatin, Dr. Matthew Jones)

Academic Support Department, Austin Peay State University   Clarksville, TN
CRLA Peer Tutor Level 1 for undergraduates   2018 - 2020

- Collaborated with director, providing both group and one-on-one tutoring for students with educational deficiencies.
- Supported courses:
  - ▸ College Algebra, Elementary Statistics, Calculus, Organic Chemistry, Algebra-based Physics, Calculus-based Physics, Anatomy and Physiology

NON-ACADEMIC EXPERIENCE

Handyman Moving Company   Nashville, TN
Sole proprietor   2014 - 2018

- My leadership and team-building skills were further honed during a break from academia, which I took to enhance my finances and fund my education. During this time, I founded and managed Handyman Moving Company, taking on the full spectrum of business operations. This role involved managing and training a team of six employees, overseeing the maintenance and scheduling of two trucks, and ensuring the highest levels of service delivery, customer satisfaction, and compliance with transportation and safety regulations. This experience not only strengthened my financial foundation but also deepened my leadership, organizational, and problem-solving skills, directly contributing to my academic and professional development.

REFERENCES

Tetyana Ignatova (Co-advisor)
Associate Professor, Nanoscience
University of North Carolina Greensboro
(336) 285-2791, t_ignato@uncg.edu

Joseph Starobin (Co-advisor)
Professor, Nanoscience
University of North Carolina Greensboro
(336) 285-2871, jmstarob@uncg.edu

Vincent H. Crespi (Mentor)
Distinguished Professor of Chemistry, Physics, and Mat. Sci. & Eng.
Director, Penn State Materials Research Science and Engineering Center
Theory Lead, Two-Dimensional Crystal Consortium, an NSF Materials Innovation Platform
Pennsylvania State University
(814) 863-0163, vhc2@psu.edu