

William Livernois

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Education

- 2020 – 2025 📖 **Ph.D. Electrical Engineering, University of Washington**
Thesis title: *Modeling Charge Transport Through Biological Molecules with Transition Metals*
- 2020 – 2022 📖 **M.S. Electrical Engineering, University of Washington**
- 2012 – 2016 📖 **B.Sc. Chemical Engineering and Physics, Massachusetts Institute of Technology**

Employment History

- 2025 – 📖 **Postdoctoral Scholar** ECE Department, UW, Seattle, WA, US
- 2020 – 2025 📖 **PhD Candidate** ECE Department, UW, Seattle, WA, US
- 2018 – 2020 📖 **R&D Engineer** GVD Corporation, Cambridge, MA, US
- 2016 – 2018 📖 **Chemical Engineer** American Boronite Corporation, Burlington, MA, US

Awards and Achievements

- Jun 2024 📖 **Arthur Chiao Global PhD Fellowship**
National Yang Ming Chiao Tung University, Hsinchu, TW
Project Title: *Atomistic Study of Random Dopant Diffusion in Silicon*
- May 2024 📖 **Session Chair, Broader Impacts Session 1**
Materials Research Society Spring Conference, Seattle, WA, US
Materials Research by the LGBTQIA+ Community and a Vision for Inclusivity
- Jul 2022 📖 **Outstanding Impact and Relevance Award**
DoD National NDSEG Fellows Conference, Boston, MA, US
Project Title: *Modeling Charge Transport Through Organometallic Biological Molecules*
- Dec 2021 📖 **Best Student Presentation Award, Session Chair**
IEEE Nanotechnology Materials and Devices Conference, Vancouver, BC, CA
Presentation: *Quantum Transport in Conductive Bacterial Nanowires*
Session Chair: *Theory and Modelling of Nanomaterials and Devices I + II*
- Sep 2020 📖 **National Defense Science and Engineering Graduate Fellow**
2022 NDSEG Fellows Conference, Boston, MA, US
Project Title: *Modeling Charge Transport in DNA Structures for Microelectronics*

Publications

- 1 **W. Livernois**, M. P. Anantram, J. J. Palacios, M. Frisch, *et al.*, “GauNEGF: Spin-dependent NEGF-DFT with Gaussian Orbitals,” 2026 (In Preparation).
- 2 **W. Livernois** and M. P. Anantram, “Spin-Dependent Hopping in Cytochromes: Role of Geometric Reorganization and Non-collinear Effects,” *Nanoscale*, 2026 (In Review).
- 3 L. Perren, **W. Livernois**, K. Woloszyn, J. Janowski, L. Faiaz, V. R. Singh, *et al.*, “Topology-Enforced Synthesis of Atomically-Precise Silver Nanoclusters in 3D DNA Lattices,” *Science Advances*, 2026 (Accepted).  DOI: 10.26434/chemrxiv-2025-3f6br-v2.
- 4 **W. Livernois**, O. Alolaiyan, A. De, and M. P. Anantram, “Scalable Force Fields for Metal-Mediated DNA Nanostructures,” *J. Chem. Theory Comput.*, vol. 22, no. 4, pp. 2000–2012, Feb. 2026, ISSN: 1549-9618.  DOI: 10.1021/acs.jctc.5c01426.

- 5 A. De, B. Lu, Y. P. Ohayon, K. Woloszyn, **W. Livernois**, *et al.*, "Transmetalation for DNA-based Molecular Electronics," *Small*, vol. 21, no. 25, p. 2 411 518, 2025.  DOI: <https://doi.org/10.1002/sml.202411518>.
- 6 **W. Livernois**, P. S. Cao, S. Saha, Q. Ding, A. Gopinath, and M. P. Anantram, "Ion detection in a DNA nanopore FET device," *Nanotechnology*, vol. 35, no. 32, p. 325 202, 2024.  DOI: 10.1088/1361-6528/ad460b.
- 7 **W. Livernois** and M. P. Anantram, "A Spin-Dependent Model For Multi-Heme Bacterial Nanowires," *ACS nano*, vol. 17, no. 10, pp. 9059-9068, 2023.  DOI: 10.1021/acsnano.2c12027.
- 8 S. Vecchioni, B. Lu, **W. Livernois**, Y. P. Ohayon, J. B. Yoder, *et al.*, "Metal-Mediated DNA Nanotechnology in 3D: Structural Library by Templated Diffraction," *Advanced Materials*, vol. 35, no. 29, p. 2 210 938, 2023.  DOI: 10.1002/adma.202210938.
- 9 **W. Livernois** and M. Anantram, "Quantum Transport in Conductive Bacterial Nanowires," in *2021 IEEE 16th Nanotechnology Materials and Devices Conference (NMDC)*, IEEE, 2021, pp. 1-5.  DOI: 10.1109/NMDC50713.2021.9677490.
- 10 D. Lashmore, P. Bystricky, **W. Livernois**, and B. Wilson, *Infrared Textile Transmitter*, US Patent 20200020224A1, Jul. 2019.  URL: <https://patents.google.com/patent/US10810868B2/en>.
- 11 A. T. Servi, E. Guillen-Burrieza, D. M. Warsinger, **W. Livernois**, K. Notarangelo, *et al.*, "The effects of iCVD film thickness and conformality on the permeability and wetting of MD membranes," *Journal of Membrane Science*, vol. 523, pp. 470-479, 2017.  DOI: 10.1016/J.MEMSCI.2016.10.008.
- 12 P. Kovacik, G. del Hierro, **W. Livernois**, and K. K. Gleason, "Scale-up of oCVD: large-area conductive polymer thin films for next-generation electronics," *Materials Horizons*, vol. 2, no. 2, pp. 221-227, 2015.  DOI: 10.1039/C4MH00222A.
- 13 **W. Livernois**, C. M. Crittenden, B. Kimbrell, F. A. Khan, A. C. Gaquere-Parker, and D. A. Stuart, "Raman Spectroscopy of Allotropes of Carbon: An Undergraduate Laboratory," *The Chemical Educator*, vol. 19, no. 2014, pp. 223-228, 2014.  URL: <http://chemeducator.org/bibs/0019001/19140223.html>.

Experience/Skills

Atomistic Modeling	 Density Functional Theory: VASP, Gaussian 16, QuantumESPRESSO Molecular Dynamics: LAMMPS, Amber (Force Field Development), VMD
Programming	 Python (PyTorch, JAX), MATLAB, FORTRAN77/90, C, Java, Excel
Continuum Modeling	 ANSYS Fluent, ANSYS Zemax, COMSOL, Sentaurus Device
Characterization	 Scanning Electron Microscopy, Scanning Probe Microscopy, UV/IR/Raman Spectroscopy, X-ray spectroscopy, Mass spectrometry
Nanofabrication	 Chemical Vapor Deposition, Physical Vapor Deposition, Photolithography, Ion Etching, Wet Etching, Ellipsometry/Profilometry, Focused Ion Beam

Teaching Experience

Jun 2026 - Jul 2026	 Program Co-lead, Chips2Future UW Study Abroad Program Taipei, TW - Co-developed first ever UW-Taiwan engineering study program - Taught transistor device section and led modeling laboratories for at NTU - Led orientations, info sessions, excursions, and site visits throughout program
Sep 2023 - Dec 2023	 Teaching Assistant, ECE Department, UW Seattle, WA, US - Provided instruction for undergraduate and graduate level photonics classes - Created new midterm modeling course project using Ansys Zemax package - Developed rubrics for all assignments and ran biweekly hybrid office hours

Teaching Experience (continued)

- Jan 2019 - Jan 2020  **Somerville High School Volunteer** Somerville, MA, US
- Weekly classroom volunteer for first period math
 - Mentored 9th and 10th grade students
- Dec 2015 - Jun 2016  **Head Lab Assistant, EECS Department, MIT** Cambridge, MA, US
- Upgraded course curriculum and developed assignment rubrics
 - Taught lectures, hired and managed lab staff
- Jan 2014 - Jun 2015  **Lab Assistant, EECS Department, MIT** Cambridge, MA, US
- Provided instruction for the introductory electronics laboratories
 - Graded lab reports and mentored students
- Jan 2012 - Jun 2012  **Teaching Assistant, Chem Dept, Univ. West Georgia** Carrollton, GA, US
- Assisted instruction of the general chemistry laboratory
 - Graded lab reports and tutored undergrad students, while in high-school

Conference Presentations

Oral Presentations

- **William Livernois**, M. P. Anantram. (2026, Mar) *Capturing non-collinear spin effects in molecular devices with gaussian basis sets* American Chemical Society Spring Meeting, Atlanta, GA, US
- **William Livernois**, M. P. Anantram. (2025, Mar) *Modeling Non-collinear Spin Transport in Cytochromes* American Physical Society March Meeting, Anaheim, CA, US
- Purun (Simon) Cao, **William Livernois**, Quanchen Ding, Soumyadeep Saha et al. (2024, Apr) *Ion Detection in a DNA Nanopore FET Device* Materials Research Society Spring Conference, Seattle, WA, US
- **William Livernois**. (2024, Apr) *Materials Science in The Anthropocene: Learning from Queer Advocacy* Materials Research Society Spring Conference, Seattle, WA, US
- **William Livernois**, M. P. Anantram. (2023, Nov) *Modeling Spin Transport in Multi-Heme Cytochromes* Materials Research Society Fall Conference, Boston, MA, US
- Simon Vecchioni, Brandon Lu, **William Livernois**, Chufan Yang et al. (2023, Nov) *Metal-Mediated Molecular Electronics in DNA Nanosystems* Materials Research Society Fall Conference, Boston, MA, US
- **William Livernois**, M. P. Anantram. (2021, Dec) *Quantum Transport in Conductive Bacterial Nanowires* IEEE 16th Nanotechnology Materials and Devices Conference (NMDC), Vancouver, BC, CA

Poster Presentations

- **William Livernois**, M. P. Anantram. (2025, Mar) *Quantum Transport in Biological Materials: Interface Effects and Spin-Dependent Phenomena in Cytochrome Systems* NIST Quantum Matters in Materials Science Workshop, Rockville, MD, US
- **William Livernois**, M. P. Anantram. (2024, Apr) *Spin Transport Modeling in The Small Tetraheme Cytochrome* Materials Research Society Spring Conference, Seattle, WA, US
- **William Livernois**, M. P. Anantram. (2021, Dec) *Late News: Modeling Quantum Transport in Bacterial Nanowires for Nanoelectronics* Materials Research Society Fall Conference, Boston, MA, US
- **William Livernois**, Scott Morrison, William O'Shaughnessy. (2019, Dec) *A Study of Initiated Chemical Vapor Deposition (iCVD) Siloxane Thin-Film Conformality at Different Length Scales* Materials Research Society Fall Conference, Boston, MA, US

- Christopher Crittenden, **William Livernois**, Joanna Denton. (2012, Mar) *Selective Binding of Halide Ions to Valinomycin via ESI-MS, NMR and DFT* National Conference of Undergraduate Research, Ogden, UT, US

Invited Lectures

- Jul 2026  **Institute of Chemistry Colloquium**
Academia Sinica, Taipei, TW
Lecture Title: *Spin-dependent Electron Transport in Multi-Heme Cytochromes: A DFT and NEGF Study*
- Jun 2026  **Energy Science Institute Hosted Seminar**
Yale University, New Haven, CT, US
Lecture Title: *Spin-dependent Electron Transport in Cytochromes: Unraveling Quantum Behavior in Heme Nanowires from First Principles*
- Nov 2025  **LBNL Molecular Biophysics & Integrated Bioimaging Seminar**
Lawrence Berkeley National Laboratory, Berkeley, CA, US
Lecture Title: *Scalable Force Fields for Metal Mediated DNA Nanostructures*
- Jul 2023  **IEEE Nano Undergrad Science Colloquium Webinar**
Több University of Economics and Technology Ankara, TR
Lecture Title: *Modeling Biomolecules in Nanodevices*
- Jan 2023  **EE 280 Exploring Devices**
University of Washington Seattle, WA, US
Lecture Title: *Modeling DNA-based Nanodevices*
- Nov 2021  **EE 200 Undergraduate Research Exploration Seminar**
University of Washington Seattle, WA, US
Lecture Title: *How Does Electrical Current Flow in DNA?*
Co-presenter with Professor Hashem Mohammad

Industry Experience

- Sep 2020 –
Sep 2021  **Marine Permaculture Consultant, Carbonwave Boston, MA, US**
- Designed seaweed permaculture arrays for carbon sequestration/drawdown
- Worked with team of engineers to model operating costs and efficiency
- Used OpenFOAM to model propulsion dynamics of floating array
- Sep 2018 –
Aug 2020  **R&D Engineer, GVD Corporation Cambridge, MA, US**
- Developed chemical vapor deposition (CVD) processes for electronics applications
- Patterned coatings and built microscale testing devices at nanofabrication facilities
- Designed and implemented environmental testing tools and quality control software
- Characterized coatings using tools including microscopy and spectroscopy methods
- Authored funding proposals for private companies and Phase I SBIR grants
- Jan 2016 –
Aug 2018  **Chemical Engineer, American Boronite Corporation Burlington, MA, US**
- Designed, built, and optimized fuel synthesis process to match downstream processing
- Optimized fuel injection for continuous boron nitride nanotube (BNNT) synthesis
- Modeled fluid dynamics and heat transfer for processes using multi-physics packages
- Used/maintained lab tools including SEM, Raman spectrometer, 4-point ohmmeter
- Managed laboratory area implementing safety protocols and managing waste streams
- Jun 2015 –
Aug 2015  **R&D Engineering Intern, Hewlett Packard San Diego, CA, US**
- Developed software package for high-speed imaging of thermal inkjet nozzles
- Analyzed fluid dynamics and designed metrics for determination of fluid properties
- Worked with fluidics team to develop new nozzle architectures

Research Experience

- Jun 2025 – Present **Postdoctoral Scholar, ECE Department University of Washington**
Seattle, WA, US
- Developed gauNEGF and G3NAT software packages for modeling molecular devices
 - Optimized HPC software packages using PyTorch and JAX frameworks
 - Modeled light-matter interactions in DNA-coordinated Ag nanoclusters
- Sep 2020 – May 2025 **PhD Researcher, ECE Department University of Washington**
Seattle, WA, US
- Developed novel spin-dependent models for cytochrome electron transport
 - Modeled electronic properties of metal-modified DNA structures in collaboration
 - Molecular modeling of biological molecules using ab-initio DFT and MD tools
 - Matched theory and modeling results with experimental results from collaborators
- Jun 2024 – Aug 2024 **Chiao Global Exchange Fellow, National Yang Ming Chiao Tung University**
Hsinchu, Hsinchu County, TW
- Research exchange with Professor Hiroshi Watanabe in the ECE Department
 - Applied atomistic models to random dopant diffusion in silicon nanostructures
 - Presented findings and mentored students modeling nanodevices
- Jun 2015 – Aug 2015 **Undergraduate Researcher, Institute for Soldier Nanotechnologies at MIT**
Cambridge, MA, US
- Used initiated CVD to develop hydrophobic coatings for membrane distillation
 - Designed experiments for characterization and testing of membranes
 - Co-authored multiple publications (Material Horizons, Journal of Membrane Science)
- Jun 2013 – Aug 2013 **Research Assistant, ChemE Department, Indian Institute of Science**
Bangalore, Karnataka, IN
- Research Exchange funded by the MISTI-India program
 - Applied rheometry techniques to amorphous calcium carbonate phases
 - Optimized the lifetime and synthesis of amorphous calcite nanoparticles
- Oct 2012 – Jun 2013 **Undergraduate Researcher, Strano Group at MIT**
Cambridge, MA, US
- Explored the use of fluorescent single walled nanotubes (SWNT) as a biosensor
 - Used boronic acid polymers to increase fluorescence in the presence of sugars
 - Constructed experimental matrices and analyzed IR and UV-vis spectroscopy data
- Oct 2011 – Jun 2012 **Research Assistant, Department of Chemistry, University of West Georgia**
Carrollton, GA, US
- Examined halide ions binding to valinomycin using mass spectrometry and NMR
 - Presented findings at the 2012 National Conference for Undergraduate Research

References

Available on Request