

# Matthew Ryan Hart

## Curriculum Vitae

### Contact Information

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Google Scholar: <https://scholar.google.com/citations?user=UP0l5jIAAAAJhl=en>

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### Personal Statement

I am a creative and interdisciplinary researcher with a passion for combining artificial intelligence with the natural sciences. My background showcases mathematical, computational, experimental, and scientific literacy, being proficient in Python, C++, and UNIX operating systems; alongside hands-on experience in organic materials and experimental methods. My tenure in academia and industry showcases my versatile skill set and global perspective. My journey reflects not just a quest for knowledge, but a passionate endeavor to contribute meaningfully to the scientific community and society at large. My strong work ethic, commitment to high ethical standards, and broad curiosity drive my pursuit of excellence and innovation in research.

### EDUCATION

#### ***B.A. Physics***

2019

North Carolina State University

Minor in Biological Sciences

Society of Physics Students at North Carolina State University

International Village at North Carolina State University

#### ***Doctor of Philosophy, Materials Science***

May 2025

University of North Carolina at Chapel Hill

Computational Linguistics Program

Graduate Student Association at The Department of Applied Physical Sciences

Science Policy Advocacy Group

**Doctoral Thesis Title: Development of Intelligent Systems for Organic Materials Engineering.**

### RESEARCH INTERESTS

Materials Informatics, Machine Learning, Computational Materials Science, Knowledge Graphs, Cheminformatics, Natural Language Processing, Language Models, Automated Science, Artificial Intelligence for Science, Ontology Engineering, Knowledge Engineering, Polymer Engineering, Dye Science.

## RESEARCH AND PROFESSIONAL EXPERIENCE

### Visiting PhD Student

May. 2024-Mar. 2025

Schwaller Group, laboratoire d'intelligence artificielle en chimie (LIAC)

École Polytechnique Fédérale de Lausanne (EPFL)

Lausanne, Switzerland

Mentor: Philippe Schwaller

- Currently integrating knowledge representation and reasoning with large language models for the creation of domain-specific intelligent systems.

### Consultant

May. 2022-2025

Ontochem, GmbH

Halle (Saale), Germany

Mentor: Lutz Weber

- Developed interactive python application to create polymer ontologies and databases.
- Utilized research in computational chemical representation to establish polymer database for use in commercial products.
- Created polymer ontology for use in commercial rule-based annotation services.
- Utilized scientific literature and patents for a variety of machine learning and natural language processing tasks.
- Utilized ontology-based annotation to create machine-readable knowledge bases.
- Participated in early-stage integration of open source large language models into commercial software.

### Graduate Research Assistant

Apr. 2021-Present

Molecular Modelling Laboratory, UNC Chapel Hill

Chapel Hill, NC

Eshelman School of Pharmacy

Dept. of Applied Physical Sciences

Faculty Mentor: Alexander Tropsha

- Used active machine learning techniques to optimize experimental design. Emphasis was placed on amorphous materials, dye development, and polymer engineering.
- Designed large, open source databases focused on organic dyes and polymer engineering.
- Developed and deployed machine learning models for predicting fitness of molecules for industrial applications.
- Developed machine learning models for the prediction of optical properties of organic molecules.

- Developed data curation pipelines for creating and managing scientific organic materials databases.
- Developed active Gaussian process models for automated catalysis studies.
- Developed large language model-based systems for autonomous research into chemical problems.
- Developed large knowledge graphs linking various materials concepts and properties.
- Led data management strategies for several academic projects.

#### **Graduate Research Assistant**

Freeman Lab, UNC Chapel Hill  
 Dept. of Applied Physical Sciences  
 Faculty Mentor: Ronit Freeman

Jan. 2020-Feb. 2021  
 Chapel Hill, NC

- Used click-chemistry to develop synthetic bio-polymeric systems based off the cellular cytoskeleton.
- Used various microscopy techniques to investigate self-assembling mechanisms of biomimetic systems.
- Developed load bearing, bio-compatible, nano-particles for drug delivery systems.

#### **Undergraduate Research Assistant**

Biomolecular Materials Group, NC State University  
 Dept. of Materials Science and Engineering  
 Faculty Mentor: Thomas LaBean

Jun. 2017-Jan. 2020  
 Raleigh, NC

- Designed RNA and DNA origami using biomolecular design software.
- Conducted initial experiments in the development of an RNA-based anticoagulant.
- Developed carbon nanotube-DNA origami for self assembling electrical structures.
- Developed methods of making carbon nanotube-integrated hydrogels for electronic device development.
- Manufactured aerogels made of biological materials with for advanced material engineering.

#### **Guest Researcher**

Andersen Lab, Aarhus University  
 Interdisciplinary Nanoscience Center (iNANO)  
 Faculty Mentor: Ebbe S. Andersen

May. 2018-Aug. 2018  
 Aarhus, Denmark

- Utilized molecular dynamics simulations and gel electrophoresis to optimize thrombin binding affinity to RNA aptamers.

## **VOLUNTEER EXPERIENCE & CAUSES**

**Volunteer Scientist**

Skype a Scientist

Jan. 2021-Jan. 2023

Virtual, Worldwide

- Participated in Skype sessions with k-12 classrooms with purpose of presenting cutting edge-research within the students' field of interest.
- Acted as guest lecturer for a variety of k-12 classrooms.

**Treasurer**

Applied Physical Sciences Graduate Student Association

May. 2021-May. 2023

Chapel Hill, North Carolina

- Organized professional development workshops for graduate students.
- Organized and maintained a yearly budget for activities related to the graduate student association.
- Part of team that successfully negotiated a pay raise for the graduate student body of the department of applied physical sciences.

**Secretary**

Science Policy Advocacy Group at UNC Chapel Hill

May. 2021-May. 2022

Chapel Hill, NC

- Organized Graduate Policy and Research Expo (GRaPE). Provided a platform for graduate students to discuss the societal impacts of their research.
- Organized workshops for writing short and effective science policy memos.
- Wrote science policy memos presented to the graduate student organization of UNC Chapel Hill.

**Graduate Student Mentor**

Molecular Modeling Laboratory

May. 2021-Present

Chapel Hill, North Carolina

- Mentored junior graduate students into developing their critical thinking, presentation, writing, and overall scientific skills.
- Guided undergraduate science students into developing foundational skills in scientific research.

**TEACHING EXPERIENCE****Graduate Teaching Assistant**

Dept. of Applied Physical Sciences, UNC Chapel Hill

Supervisor: Richard Goldberg, Glenn Walters

Aug. 2020-May. 2021

Chapel Hill, NC

- APPL110 Intro to Design and Making

2020-2021 Academic Year

### Graduate Teaching Assistant

Dept. of Physics, UNC Chapel Hill

Supervisor: Duane Deardorf, Daniel Young

Summer 2021

Chapel Hill, NC

- PHYS 215 Physics for Life Sciences II

2021 Summer Session

## HONORS, AWARDS & MEMBERSHIPS

Shared 2nd place overall and Audience choice award as part of North Carolina State University's team at the international biomolecular design competition BIOMOD 2018, held at the University of California, San Francisco.

## PUBLICATIONS

Abhichart Krissanaprasit, Carson Key, Michael Fergione, Kristen Froehlich, Sahil Pontula, **Matthew Hart**, Pedro Carriel, Jørgen Kjems, Ebbe Sloth Andersen, Thomas H. LaBean. "Genetically Encoded, Functional Single-Strand RNA Origami: Anticoagulant" <https://doi.org/10.1002/adma.201808262>. April 2019.

**Matthew Hart**, Kelvin Idanwekhai, Vinicius M. Alves, Alexander J. M. Miller, Jillian L. Dempsey, James F. Cahoon, Chun-Hsing Chen, David A. Winkler, Eugene N. Muratov, and Alexander Tropsha "Trust Not Verify? The Critical Need for Data Curation Standards in Materials Informatics" *Chemistry of Materials* 2024 *36* (19), 9046-9055 DOI: 10.1021/acs.chemmater.4c00981

Geemi Wellawatte, Huixuan Guo, Magdalena Lederbauer, Anna Borisova, **Matthew Hart**, Marta Brucka, Philippe Schwaller "ChemLit-QA: A human evaluated dataset for chemistry RAG tasks" *AI for Accelerated Materials Design - NeurIPS 2024* <https://openreview.net/forum?id=6PoHvQeeHU>

Alexandru Oarga, **Matthew Hart**, Andres M Bran, Magdalena Lederbauer, Philippe Schwaller "Scientific Knowledge Graph and Ontology Generation using Open Large Language Models", *AI for Accelerated Materials Design - NeurIPS 2024* <https://openreview.net/forum?id=wMMhffCxXZ>

In Preparation:

**Under Review** *Machine Learning Reject Option for Increased Accuracy in Predicting Optical Properties* James Wellnitz, Kathryn Kirchoff, Marielle Rath, Travis Maxfield, **Matthew Hart**, Konstantin Popov, Alexander Tropsha. Expected to be published 2024.

*Aurora: Machine Learning Tool for the Discovery and Design of Organic Compounds for Optical Applications* **Matthew Hart**, James Wellnitz, Kelvin Idanwekhai, Stephen Boyer, Lutz Weber, Konstantin Popov, Alexander Tropsha. Expected to be published 2024.

*Ontologies as Antipsychotics for Domain-Specialized LLM Systems* **Matthew Hart**, Kelvin Idanwekhai, Ishaan Balakrishnan, Lutz Weber, Claudia Bobach, Stephen Boyer, Alexander Tropsha. Expected to be published 2024.

*Discovery of Chemical Quantitative Structure-Use Case Relationships* **Matthew Hart**, Kelvin Idanwekhai, Jon-Michael Beasley, Nyssa Tucker, James Wellnitz, Stephen Boyer, Lutz Weber, Eugene Muratov, Philippe Schwaller, Alexander Tropsha. Expected to be published 2024.

**Under Review** *Informatics for the Discovery of Organic Materials* **Matthew Hart**, Kelvin Idanwekhai, Eugene Muratov, David Winkler, Alexander Tropsha. Expected to be published 2024.

## PRESENTATIONS

**Matthew R. Hart** "DNA-Wrapped Carbon Nanotubes as a Platform for Neuromorphic Memristor-Based Reservoir Computing" Poster. Presented at Carolina Science Symposium 2019. Raleigh, NC, USA.

**Matthew R. Hart** "The development of the DataCHASE Interactive Molecular Database". Presented at Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE) 2021. Chapel Hill, NC, USA.

**Matthew R. Hart** "Active Machine Learning for the Discovery of Novel Catalysts". Presented at UNC seminar for the department of applied physical sciences 2022. Chapel Hill, NC, USA.

**Matthew R. Hart** "Machine Learning for the Discovery and Optimization of Organic Dyes". Presented at The American Physical Society's March Meeting 2024. Minneapolis, MN, USA.

**Matthew R. Hart** "Polymer Re-purposing Using an LLM-Ontology Hybrid System ". Presented at The American Chemical Society's Spring Conference 2024. New Orleans,

LA, USA.

## LANGUAGES

### **English**

Native Speaker

### **German**

Intermediate Speaker

### **French**

Novice Speaker

## References

### ***Dr. Alexander Tropsha***

Academic Advisor

alex.tropsha@unc.edu

### ***Dr. Eugene Muratov***

Academic Co-Advisor

murik@email.unc.edu

### ***Dr. Lutz Weber***

Academic Mentor

lutzweber.lw@gmail.com

### ***Dr. Stephen Boyer***

Collaborator

skboyer@gmail.com

### ***Dr. Philippe Schwaller***

Academic Mentor

philippe.schwaller@epfl.ch

### ***Dr. Claudia Bobach***

Academic Mentor

c.bobach@digital-science.com