Matthew Hart, PhD

Materials Scientist | AI/ML Researcher

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Birth Year: 1997

Interdisciplinary researcher with 5+ years developing AI/ML systems for chemical and materials applications. Expert in knowledge engineering, cheminformatics, and autonomous research platforms. Proven track record delivering production systems for chemical and pharmaceutical projects.

Technical Skills

Programming: Python, C++, UNIX/Linux, Git, Docker
ML/AI: PyTorch, Generative AI, scikit-learn, Active Learning, Gaussian Processes, LLMs, LangChain, RAG, NLP
Cheminformatics: RDKit, Molecular Dynamics, QSAR/QSPR, High-throughput Screening
Data Engineering: Knowledge Graphs (Neo4j, RDF), Ontologies (OWL), SQL, NoSQL
Domain: Materials Informatics, Polymer Science, Organic Chemistry, MOFs, Drug Discovery

Professional Experience

Postdoctoral Researcher | EPFL *Nov 2025 – Present*
Laboratory for AI in Chemistry, Lausanne, Switzeralnd

- Developing ML models for metal-organic framework design targeting carbon capture applications
- Integrating domain knowledge with deep learning for accelerated materials discovery

AI/ML Consultant | Ontochem GmbH *May 2022 – May 2025*
Halle (Saale), Germany

- Built commercial polymer ontology system deployed in production serving pharmaceutical clients
- Developed Python application automating ontology creation, reducing manual curation time by 70%
- Engineered NLP pipelines processing 100K+ scientific documents for knowledge extraction
- Led integration of open-source LLMs into commercial chemistry software platform

Graduate Research Assistant | UNC Chapel Hill *Apr 2021 – Aug 2025*
Molecular Modeling Laboratory, Eshelman School of Pharmacy

- Built open-source databases with 50K+ curated compounds and standardized data pipelines
- Created ML models predicting molecular properties with $R^2 > 0.85$ for industrial applications
- Designed autonomous research system using LLMs for hypothesis generation and experimental planning
- Developed knowledge graph (500K+ entities) integrating chemical literature and experimental data

Education

Ph.D. in Materials Science | University of North Carolina at Chapel Hill *2020 – 2025*
Dissertation: Development of Intelligent Systems for Organic Materials Engineering

B.A. in Physics (Minor: Biological Sciences) | NC State University *2015 – 2019*

Selected Achievements & Publications

- **Digital Discovery 2026:** "Scientific knowledge graph and ontology generation using open large language models"
- **Chemistry of Materials 2024:** "Trust Not Verify? Critical Need for Data Curation Standards"
- **NeurIPS 2024 (AI4Mat):** ChemLit-QA dataset for chemistry RAG; Scientific knowledge graphs with LLMs
- **Advanced Materials 2019:** Genetically encoded RNA origami anticoagulant
- **Awards:** 2nd Place BIOMOD 2018 (international biomolecular design competition)

Languages & Leadership

Languages: English (native), German (intermediate), French (novice)

Leadership: Treasurer, Graduate Student Assoc. (2021–23)
Mentor, 10+ graduate/undergraduate students (2020–25)