Magnus Strandgaard

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Summary

Computational chemist turned data and cloud engineer. PhD in computational chemistry with a track record of end-to-end Python/ML systems for generative molecular design and property prediction, paired with enterprise cloud experience (AWS, Terraform, CI/CD) supporting a 1M+ user application. Driven by a strong passion to build computational systems that accelerate the green energy transition and healthcare.

Experience

Netcompany, **Linux and Cloud Operations Engineer** — Copenhagen, DK — 2025 – present

- Maintained and extended the AWS infrastructure for a **1M+ user application across 11 environments** (10 dev replicas + production), defining compute, networking, and data resources as code in Terraform with per-environment workspaces and AWS SSO access.
- Became the team's **lead Terraform developer within 3 months** of joining. Led the zero-downtime migration of an enterprise solution (1,000+ live resources) to a managed Terraform state, establishing rigorous code review practices and mitigating edge cases for seamless production deployment.
- Developed and maintained automated **CI/CD** pipelines in Azure DevOps and Jenkins, integrating strict policy checks and testing to ensure high-quality, production-ready code delivery.
- Python development for automation of internal processes, including ingestion and processing of critical data. Engineered a robust **Python data-processing pipeline** that replaced a legacy service, resolving performance bottlenecks and **reducing cloud spend by ~$3,500/month** while ensuring secure data handling.

Dept. of Chemistry, University of Copenhagen, **Postdoctoral Researcher** — Copenhagen, DK — 2024 – 2025

- Designed and operated **data pipelines across 4 HPC clusters** to ingest, curate, and validate **100K+ molecular records** from the Cambridge Structural Database, enabling **structure-property analysis** of transition-metal complexes.
- Built **ML workflows** combining molecular fingerprints and **graph neural networks** to predict chemical properties of 3D structures, with accuracy gains over baseline models. Orchestrated distributed GPU training via **SLURM** and the WandB **MLOps** tool.
- Developed a novel **synthetic accessibility scoring tool** in **Python with C++ bindings** for generative molecular design pipelines.

Dept. of Chemistry, University of Copenhagen, **PhD Researcher** — Copenhagen, DK — 2021 – 2024

- Developed end-to-end **in silico molecular discovery pipelines** coupling quantum chemistry with **generative ML models** (genetic algorithms, variational autoencoders) for **catalyst design and compound optimization**, screening thousands of candidates with **RDKit, Pandas, and SQLite**.
- Collaborated with the **University of Oslo** theoretical chemistry group to implement a **variational autoencoder (VAE)** for molecular inverse design, training **PyTorch** models on HPC GPUs to generate novel transition-metal complexes.
- Served as **HPC cluster administrator** for the physical chemistry department (**50+ active users**), managing Linux environments, SLURM job scheduling, and **reproducible computational workflows**.
- Created and maintained **4 open-source research repositories** on GitHub as lead developer.
- Mentored **60+ undergraduate students** as teaching assistant for physical chemistry and mathematics courses.

Dept. of Energy, Technical University of Denmark, **Research Assistant** — Kongens Lyngby, DK — 2021 – 2021

- Implemented a **Message Passing Neural Network (MPNN)** in **PyTorch** to predict forces and energies of magnesium battery cathode candidates, enabling **molecular dynamics simulations** of next-generation energy-storage materials.

Education

PhD	**University of Copenhagen**, Computational Chemistry	2021 – 2024
MSc	**Technical University of Denmark**, Physics and Nanotechnology	2018 – 2021
BSc	**Technical University of Denmark**, Physics and Nanotechnology	2015 – 2018

Skills

Languages & Engineering: Python (Expert) · FastAPI · REST APIs · Unit Testing (Pytest) · SQL & NoSQL (RDS/DynamoDB) · Git · Docker · CI/CD · Familiar with: TypeScript, React, Svelte, Tailwind, C++, Golang

Data Science & ML: PyTorch · Scikit-learn · SciPy · NumPy · Pandas · MLOps (WandB, MLflow) · Familiar with: LangChain, dbt

Scientific Visualization: Streamlit · Plotly · Matplotlib

Cloud & Platform: AWS (Full Stack) · Terraform · SLURM (HPC admin) · Proxmox · Ansible · Jenkins · Azure DevOps · Linux · Familiar with: Kubernetes, Nextflow, Apache Airflow, Azure

Computational Chemistry: RDKit · Molecular Embeddings · QSPR/QSAR · ORCA · xTB · VASP · ADF

AI-Assisted Development: Claude Code · Claude Design · Gemini CLI · GitHub Copilot · building and shipping production software with AI coding agents

Spoken: Danish & Norwegian (native) · English (fluent) · Spanish (basic)

Publications

A Deep Generative Model for the Inverse Design of Transition Metal Ligands and Complexes 2025
Magnus Strandgaard, Linjordet T, Kneiding H, Burnage AL, Nova A, Jensen JH, Balcells D
10.1021/jacsau.5c00242 (JACS Au)

Discovery of molybdenum-based nitrogen fixation catalysts with genetic algorithms 2024
Magnus Strandgaard, Seumer J, Jensen JH
10.1039/D4SC02227K (Chemical Science)

Genetic algorithm-based re-optimization of the Schrock catalyst for dinitrogen fixation 2023
Magnus Strandgaard, Seumer J, Benediktsson B, Bhowmik A, Vegge T, Jensen JH
10.7717/peerj-pchem.30 (PeerJ Physical Chemistry)

SMILES All Around: Structure to SMILES conversion for Transition Metal Complexes 2025
Rasmussen MH, **Magnus Strandgaard**, Seumer J, Hemmingsen LK, Frei A, Balcells D, Jensen JH
10.1186/s13321-025-01008-1 (Journal of Cheminformatics)

Projects

Self-hosted Proxmox Homelab

- Deploy and maintain a self-hosted **Proxmox** server orchestrating multiple VMs and LXC containers for web and IT services on Linux, with provisioning and configuration **automated via Ansible and Terraform**.

Full-stack AWS-hosted Web Application

- Engineered a **full-stack web application** (**React/TypeScript/Tailwind** frontend, **Python/FastAPI** backend) on a near-zero-cost serverless AWS environment in Terraform, directing the implementation with Claude Code. Live at mcgamertime.drmaggi.com.

Shopify E-Commerce Platform

- Built and self-administer a live **Shopify** e-commerce store end-to-end, including domain and user management.
- Used **Claude Code** to build a custom Shopify integration that manages the full product catalog from version-controlled **YAML** files, syncing structured product data directly to the store.