

Adil Aboobacker

DATA SCIENTIST & TECHNICAL CONSULTANT · ML & PRODUCT

(+49) 0176 60463676 | adilpsnde@gmail.com | adil-aboobacker-601903202



Professional Profile

PhD researcher with a strong background in computational modelling, data analysis and software development, combined with hands-on experience in industrial energy optimization. I build Python-based analytical workflows, apply machine learning, and translate complex technical problems into practical software and data solutions. I am particularly interested in applying these skills to digitalization, data-driven optimization and technology development within the energy industry.

Skills

Data Science	Python (NumPy, pandas, scikit-learn), ML, model fine-tuning, PCA & dimensionality reduction, statistical analysis, time-series forecasting
Software & Engineering	Workflow automation, HPC & GPU computing, Bash, data integration (sensors/MQTT/ERP/spreadsheets), Agentic coding- Claude/Codex
Product & Consulting	Customer discovery, problem validation, MVP scoping, stakeholder communication, dashboard/UX prototyping
Tools	Git, MATLAB, Power BI, SQL, REST APIs / JSON
Communication	Team-building, data visualization, scientific presentation, product pitching

Data & Computational Projects

Open-Source Workflow for Automated Reaction Discovery in Battery Electrolytes (EnsembleMTD)

HELMHOLTZ INSTITUTE MÜNSTER / UNIVERSITY OF MÜNSTER

Münster, Germany
Nov. 2022 - 2025

- Built an end-to-end Python workflow that couples enhanced-sampling simulations with automated reaction-network analysis to extract reaction pathways directly from raw trajectory data.
- Designed the pipeline to aggregate ensembles of independent runs into ranked, reproducible product candidates.
- Ran a systematic parameter screen to define robust default settings, making the tool reusable across different chemical systems
- First-author manuscript, unpublished. Code: <https://github.com/adilpsn/EnsembleMTD>

Machine-Learning Force Field via Foundation Model Fine-Tuning

HELMHOLTZ INSTITUTE MÜNSTER / UNIVERSITY OF MÜNSTER

Münster, Germany
2024 - 2026

- Fine-tuned a pretrained MACE foundation model (a machine-learning force field) on self-generated DFT data to obtain a fast, system-specific model at near-DFT accuracy.
- Used PCA on the dataset to select a diverse, non-redundant set of training structures, improving data efficiency and coverage.
- Applied the model and large-scale analysis to quantify transport, coordination, and clustering across electrolyte formulations.
- Presented related results as a poster at IMLB 2024, Hong Kong; manuscript in progress.

Simulation & Scientific Data Analysis

HELMHOLTZ INSTITUTE MÜNSTER / UNIVERSITY OF MÜNSTER

Münster, Germany
2025 - 2026

- Built reusable Python workflows to process large simulation datasets and extract quantitative metrics for comparing complex material systems.
- Integrated computational and experimental data to identify structure–performance relationships and communicate findings to cross-functional research teams.
- Analysis contributed to two peer-reviewed Angewandte Chemie publications (2025, 2026):
Angew. Chem. Int. Ed. 2025, 64, e202506826 | Angew. Chem. Int. Ed. 2026, e3797296

Entrepreneurial and Product Experience

Founding Team | Product & Data

UTILIQ — REACH EUREGIO START-UP CENTER (HEADVENTURES PROGRAM)

Münster, Germany
2026

- Co-developing UtiliQ, an early-stage industrial energy-optimization and test-bench scheduling concept for manufacturers of generators, engines, and power units.
- Ran customer discovery with industrial stakeholders and validated the core problem: poorly scheduled high-power test benches waste energy, incur grid import/export costs, and lower utilization.
- Translated the problem into a data-product MVP: data integration (sensors, MQTT, ERP, spreadsheets), live asset monitoring, generation/consumption forecasting, and schedule optimization under grid and due-date constraints.
- Pitched the product to a jury of experts on July 2026, positioning UtiliQ as a data-driven energy optimizer for sites with high testing energy throughput.

Education

University of Münster	Ph.D. in Chemistry	2022-Present	Münster, Germany
IISER Thiruvananthapuram	BS-MS Chemistry, Minor Physics 7.8 CGPA	2017 - 2022	Kerala, India

Conferences

Poster Presentation: Computational Study of Anions in High-Concentration Electrolytes	Hong Kong
INTERNATIONAL MEETING ON LITHIUM BATTERIES (IMLB)	16-21 Jun. 2024
Presented machine-learning and simulation analysis of ion transport, coordination, and decomposition trends in high-concentration electrolytes to an international audience.	

Certifications

- Claude Academy: [Claude Code in Action](#)
- Claude Academy: [Claude Code 101](#)

Language

English: Native | German: A2 (Self-assessed)