Tarik Ammouli, Ph.D.

Computational Physical Chemist · Research Software Engineer

+33 7 82 03 90 84 tarik.ammouli@gmail.com linkedin.com/in/tarik-ammouli ORCID 0000-0002-4275-5896 tarikammouli.com

Ph.D. in physical chemistry and research software engineer, I design drug-discovery solutions alongside multidisciplinary teams. With 5+ years bridging computational science and production software, I industrialise molecular-modelling pipelines, scale them across cloud and HPC infrastructure, and translate R&D needs into technical roadmaps — convinced that an innovation is only as valuable as its economic viability.

Professional experience

Research Software Engineer, Computational Chemistry Sep 2023 – Present
Qubit Pharmaceuticals · Paris, France

- **Strategic data & AI:** designed and built the ab-initio quantum-chemistry pipeline characterising the electronic structure of thousands of compounds and producing millions of training data points for the company's foundation model, the backbone of its AI strategy for drug discovery.
- **Industrialisation at scale:** scaled structure- and ligand-based virtual screening to millions of compounds by integrating parallelised docking engines (speed and binding-score accuracy) and a Milvus vector-search database for similarity search; accelerated drug-discovery cycles through distributed compute and automated CI/CD flows.
- **Cost governance:** designed and deployed a cloud cost-control strategy (budget tracking, cost/performance arbitration) cutting infrastructure spend by 20%.
- **Cross-functional leadership:** bridge between medicinal chemists and software engineering, translating R&D needs into technical roadmaps; mentored interns and onboarded newcomers; technical support for internal users of the Atlas platform.
- **Engineering excellence:** end-to-end molecular enumeration and 3D-conformer workflows; bots automating data recovery across HPC clusters; legacy codebases refactored into maintainable services with CI/CD, automated tests, containerisation, code reviews and documentation.

Postdoctoral Researcher Apr 2022 – Aug 2023
CINaM – CNRS UMR 7325, Aix-Marseille Université · Marseille, France

- **Research strategy:** led a study on the catalytic selectivity of chiral single-walled carbon nanotubes (SWCNTs) during CCVD growth, steering the laboratory's experimental synthesis protocols.
- **Quantum modelling:** characterised SWCNT / Ni catalyst systems with DFT (VASP), quantified interfacial charge transfer with Bader analysis and described high-temperature interfaces with tight-binding models; poster at NT23 (Arcachon, June 2023).

Ph.D. Researcher in Physical Chemistry Nov 2018 – Dec 2021
IS2M – Université de Haute-Alsace (CNRS UMR 7361) · Mulhouse, France

- **Project leadership:** drove a three-year multidisciplinary project on the capture of persistent organic pollutants (POPs) by cationic zeolites in the presence of water, from molecular modelling to the synthesis of selective adsorbents — 2 peer-reviewed articles, 2 international conferences and a Best Poster Award (Young Scientist Day, IS2M, 2019).
- **Multi-scale simulation:** coupled periodic DFT, molecular mechanics and configurational-bias Monte Carlo to characterise adsorption mechanisms; screened extra-framework cations (K+, La3+, Y3+) for selective POP adsorption and derived new DFT-based force-field parameters.
- **Theory meets experiment:** performed cation-exchange syntheses (XRF-quantified) and validated models against manometry, XRD and TGA/DSC; identified a hydration threshold beyond which POP adsorption collapses, informing energy-efficient zeolite activation protocols.
- **Teaching:** thermodynamics and solid-mechanics tutorials and labs for undergraduate and postgraduate students.

Education

Ph.D. in Physical Chemistry Nov 2018 – Dec 2021
Université de Haute-Alsace – IS2M (ED 182 Physique et Chimie-Physique) · Mulhouse, France

M.Sc. in Physics & New Technologies — Major de promotion Sep 2016 – Jul 2018
Université Hassan II de Casablanca · Casablanca, Morocco

B.Sc. in Physics & Applications Sep 2013 – Jul 2016
Université Hassan II de Casablanca · Casablanca, Morocco

Honors & training

- **Best Poster Award** — Young Scientist Day, IS2M – Institut de Science des Matériaux de Mulhouse (Dec 2019)
- **CECAM Molsim20 Fellow** — Summer school on molecular simulation, Van 't Hoff Institute for Molecular Sciences, University of Amsterdam (Jan 2020)
- **Major de promotion** — M.Sc. Physics & New Technologies, Université Hassan II de Casablanca (2018)
- **M2 research internship** — IS2M, Mulhouse (Feb – Jul 2018): adsorption of bis-chlorinated isomers within dehydrated potassium-exchanged zeolites.

Languages

French (fluent) · English (fluent) · Arabic (fluent) · Spanish (basics)

Key competencies

DeepTech Strategy & Leadership

R&D to roadmap

Translating scientific needs into technical roadmaps · Product industrialisation · Scientific storytelling for non-specialists

Cross-functional alignment

Bridge between medicinal chemists and engineering · Stakeholder alignment · Mentoring interns & onboarding

Delivery & governance

Agile delivery (Asana, Jira, Notion) · Cloud cost governance (20 % lower infrastructure spend) · Managing uncertainty in R&D projects

Architecture & design

UML & ERD system design · Data architectures · Observability-driven operations

Computational Chemistry & Cloud/HPC Engineering

Languages & frameworks

Python, Go, Ruby, Fortran, Bash, SQL, FastAPI, Django, Rails, Streamlit

Cloud & data

AWS (EC2, EKS, S3, RDS, Lambda, ParallelCluster), PostgreSQL, Elasticsearch, Milvus, Redis

DevOps & CI/CD

Git, Docker, Kubernetes, Singularity / Apptainer, GitLab CI, GitHub Actions, ArgoCD

Observability & data engineering

Prometheus, Grafana, ELK Stack, Airflow

Cheminformatics & virtual screening

RDKit, ChemAxon, OpenBabel, AutoDock, Vina / VinaXB

Atomistic modelling

VASP, PySCF, GULP, Towhee, Tinker-HP

Analytics & visualisation

Materials Studio, ASE, VASPKIT, VMD, PyMOL, VESTA, DataWarrior

Selected publications

Adsorption of polychlorinated aromatics in potassium exchanged faujasite: A molecular simulation study

T. Ammouli, J. Paillaud, H. Nouali, M. Hanf, R. Stephan, P. Sonnet, I. Déroche. *Microporous and Mesoporous Materials* 2026, 413, 114272. doi:10.1016/j.micromeso.2026.114272

Insights into Water Adsorption in Potassium-Exchanged X-type Faujasite Zeolite: Molecular Simulation and Experiment

T. Ammouli, J. Paillaud, H. Nouali, R. Stephan, M. Hanf, P. Sonnet, I. Deroche. *The Journal of Physical Chemistry C* 2021, 125(35), 19405–19416. doi:10.1021/acs.jpcc.1c03593

Adsorption de dichlorobenzènes par des zéolithes cationiques en présence d'eau

Ph.D. thesis, Université de Haute-Alsace – Mulhouse (ED 182), 2022. Directors Philippe Sonnet & Régis Stephan. HAL tel-03888267

Conference contributions

Poster · A DFT study of the nanotube-catalyst charge transfer during the CVD growth

T. Ammouli, C. Bichara. NT23 – 23rd International Conference on the Science and Applications of Nanotubes and Low-Dimensional Materials, Arcachon, France, 4 – 9 June 2023.

Poster · Removal of Persistent Organic Pollutants (POPs) by cationic zeolites under humid conditions: a coupled in-silico / experimental investigation

T. Ammouli, J. Paillaud, P. Sonnet, R. Stephan, M. Hanf, I. Deroche. FEZA 2021 – 8th Conference of the Federation of European Zeolite Associations, Virtual (organised from Brighton, UK), 5 – 9 July 2021.

Oral · Influence of extra-framework cations and hydration rate on adsorption properties of polychlorinated aromatics in zeolite

T. Ammouli, J. Paillaud, P. Sonnet, R. Stephan, M. Hanf, I. Deroche. Matériaux 2022 – Conférence internationale de la Fédération Française des Matériaux, Lille, France, 24 – 28 October 2022.

Certifications

Pharma: BI for Biopharma · Pharma Industry Fundamentals · Cheminformatics & MedChem

Data & Infrastructure: AWS Cloud · Kubernetes · Apache Airflow 3 · Virtualization

Software Architecture: Data Architectures · Kibana · UML System Design