Kemal Özkırşehirli

MIT B.Sc. Candidate — Computer Science and Engineering, Physics, Applied Mathematics. Minors in Philosophy and Writing. Cambridge, MA · kemalozk@mit.edu · LinkedIn · GitHub · Google Scholar

I work at the intersection of AI/ML, physics, computational chemistry, molecular simulation, CADD, protein and genome modeling, geometric deep learning, statistical mechanics, and scientific workflow engineering. My work turns difficult scientific systems into computable representations, testable algorithms, and decision-making tools for discovery.

Education

Massachusetts Institute of Technology — Cambridge, MA B.Sc. expected May 2027. GPA: 5.0/5.0.

- Majors: Computer Science and Engineering, Physics, Applied Mathematics.
- Minors: Philosophy, Writing.
- Transferred to MIT from Columbia University.
- Graduate-level coursework: Deep Learning; Platforms for Drug Discovery; Atomistic Modeling and Simulation; Statistical Physics in Biology; Stochastic Processes.
- Undergraduate-level coursework: Design and Analysis of Algorithms; Theory of Computation; Natural Language Processing; Sublinear Time Algorithms; Computer Structures and Architectures; Intensive Python and C/C++/Assembly Programming Labs; Probability Theory and Random Variables; Linear Algebra; Quantum Chemistry; Biochemistry; Advanced Organic Chemistry; Discrete Mathematics; Genetics.
- Humanitas core: Theory of Models; Rhetoric; Language and Power; Advanced Essay; Poetry; Critical Social Theory; Political Philosophy; Memoir.

Columbia University — New York, NY B.A. study in Chemistry and Computer Science-Mathematics, Sept 2024–May 2025. GPA: 4.07/4.00.

- Received a Likely Letter from Columbia University and was named a Science Research Fellow.
- Coursework: Intensive Organic Chemistry I; Data Structures and Algorithms; Accelerated Multivariable Calculus; Mechanics and Thermodynamics; Electricity and Magnetism; Introductory Electrical Engineering and Lab.
- Core Curriculum: University Writing: Gender and Sexuality / 21W.011 Writing and Rhetoric; Literature Humanities I & II; Frontiers of Science.

Üsküdar American Academy — Istanbul, Türkiye 2019–2024. Grade: 97/100.

- Dr. Virginia Canfield Award for Overall Excellence, 2022.
- George Ripley Tracy Award for Academic Distinction, 2023.
- Graduating Academic Award in Science, 2024.

International Baccalaureate Diploma Programme — November 2023 cohort Score: 44/45.

- Higher Level: Mathematics Analysis and Approaches, Physics, Chemistry.
- Standard Level: English A Language and Literature, Turkish A Literature, Turkey in the 20th Century.
- Extended Essay in English Literature: A.

Stanford Pre-Collegiate University-Level Math and Physics — 2022–2023

- Multivariable Differential Calculus, Multivariable Integral Calculus, and Differential Equations.

Research, Industrial, and Professional Experiences

Founder and Research Lead — Methodology-First 3D Mesh Learning

Independent research collaboration — Jun 2026–Present

- Leading a 7-member international research collaboration developing a new methodology for 3D mesh and point-cloud learning rather than forcing a premature domain application.
- Building the technical roadmap around kNN graph pipelines, Point Transformer v3-style architectures, geometric representation learning, reproducible experiments, literature synthesis, and preprint-oriented manuscript planning.
- Applying the method to molecular, biological, or life-science settings if and only if the application provides a principled scientific fit for the methodology and an informative benchmark.
- Coordinating weekly technical meetings, literature presentations, experimental milestones, contributor responsibilities, documentation, and manuscript preparation.

Machine Learning Engineer — Chromosomal Protein Folding / ChromoGen-V2

MIT CSAIL / MIT Chemistry, Zhang and Kellis Groups — May 2026–Present

- Developing ChromoGen-Engine V2, a conditional diffusion and evaluation pipeline for small-molecule-perturbed single-cell 3D chromatin generation.

- Building a data engine integrating Plate-C / Easy Dip-C treatment structure data with CHARM-style same-cell Hi-C, RNA-seq, ATAC-seq, and histone-modification data.
- Designing structure-grounded benchmarks for generated chromatin ensembles: held-out distance/contact agreement, P(s) decay, condition separation, ensemble coverage, calibration, failure-mode analysis, and sequence/regulatory attribution.

AI/ML, Inference, and Optimization Engineer — Autoimmune Target Discovery

*Experimental Drug Development Centre, ASTAR; Dr. Sun and Dr. Cai** — Apr 2026–Present

- Architecting V2M-Engine, a calibrated genetics-to-mechanism target-discovery framework for autoimmune disease.
- Mapping GWAS and fine-mapped risk variants onto regulatory programs, causal immune cell states, and targetable disease mechanisms using single-cell foundation models, QTL/colocalization evidence, and known therapeutic targets as embedded validation controls.
- Developing a modular sequence-to-cell-state-to-targetability engine coupling variant-effect scoring, Perturb-seq validation, counterfactual immune-state transport, and structure/affinity-aware target prioritization.

PRISM AI Safety Fellow — Protein Foundation Model Red-Teaming and Evaluation

PRISM, W2D2, Siemens — May 2026–Present

- Selected from 800+ applicants for PRISM 2026 to develop adversarial evaluation methods for protein foundation models.
- Testing when biologically plausible outputs fail sequence-structure-function constraints, uncertainty calibration, developability, model-claimed mechanisms, and protein-design reliability checks.
- Building safety-bounded benchmarks and failure taxonomies using prior work in EVEdesign, A*STAR V2M, antibody/protein models, CADD, and uncertainty-aware candidate ranking.

Algorithm Design, Engineering, and Optimization — Functional Protein Discovery

EVEdesign, Harvard Medical School / collaborative project — Apr 2026–Present

- Contributing to EVEdesign, an open-source, method-independent protein-design platform across a 21-person, 18-institution, 8-country collaboration.
- Developing uncertainty-aware candidate selection, sequence-structure-function objective integration, protein-language-model/evolutionary-prior scoring, and agent-based tool orchestration for scalable lab-in-the-loop biosequence design.

Student Principal Investigator — Özkırşehirli Group and TBXT Small-Molecule Hackathon

MIT, Pillar VC, onepot — Apr 2026–Present

- Leading an 11-person chordoma-focused TBXT/brachyury computational hit-identification sprint targeting PDB 6F59 chain A / TBXT G177D site F.
- Compressed 2,274 prior-art compounds plus 737 raw analogs into 503 filtered analogs plus 30,000 BRICS recombinations, then into a 570-compound novelty-filtered pool.
- Integrated Vina ensemble docking, GNINA CNN pose/pKd scoring, Vina-trap detection, RF/XGBoost TBXT QSAR, Boltz-2 co-folding, MMGBSA/FEP scaffolding, T-box paralog selectivity, Rowan IC50/affinity analysis, RDKit descriptors/BRICS, onepot/muni catalog checks, and Bash/HPC automation.
- Prioritized a 570 → 137 strict-pass → 24 submission-ready → 4 judge-facing site-F funnel under sourceability, lead-likeness, PAINS/forbidden-motif, selectivity, cost, chemistry, and supplier-risk gates.

LLM/NLP, Statistical Mechanics, and Theoretical Chemistry Researcher

Columbia University, Prof. David Reichman — Jan 2026–May 2026

- Developed ChemAgent-QSM, an LLM-guided agentic framework converting natural-language chemistry prompts into validated PySCF quantum-chemical workflows.
- Generated auditable Python workflows for time-correlation functions, local-order metrics, relaxation timescales, mobility fields, structure/dynamics coupling, optimized geometries, electronic-structure descriptors, and vibrational spectra.
- Developed LLM-trajectory features and ML analysis workflows for dynamical heterogeneity in glass-forming and other systems, including mean squared displacement, SISFs, and MSCOPE baselines.

Project Co-Lead — Deep Reinforcement Learning for Antibody-Antigen Interactions

AI@MIT / AIM Labs — Jan 2026–May 2026

- Co-led a six-person team developing a structure-informed cross-attention transformer and ESM-2 pipeline mapping protein/pathogen sequences to candidate antibodies.
- Curated datasets from OAS, SAbDab, IEDB, and CoV-AbDab-style sources.

- Reduced training time by approximately 40% using PPO-based reinforcement learning against AlphaFold-Multimer/IGFold structural metrics and GPU-distributed PyTorch DDP on MIT SuperCloud.

Teaching Fellow and Grader — 6.1200[J] Discrete Mathematics / Mathematics for Computer Science

MIT EECS — Jan 2026–Present

- Selected after receiving an A+ and ranking in the top 1% of students enrolled in MIT EECS's largest foundational theoretical computer science course.
- Supporting a 250+ student cohort through recitations, office hours, proof-intensive grading, midterms, and finals in logic, graph theory, recurrence relations, asymptotic analysis, and cryptography.

AI/ML for Statistical Mechanics Simulations Researcher and Teaching Fellow

MIT Physics, Prof. A. Nihat Berker — Jan 2022–Present

- Invited to conduct research after ranking within the top 1% in Prof. Berker's graduate-level 8.334 Phase Transitions and Renormalization-Group Theory while in high school.
- Building a machine-learning-augmented Kadanoff renormalization-group framework using PyTorch and a graph neural network spin classifier to identify fixed points and phase boundaries in spin-1/2 antiferromagnetic systems.
- Mentored 200+ students on college applications, decisions, and career paths while teaching augmented chemistry and classical/quantum mechanics condensed courses.

Head of Chemistry Research-Implementation / Backend Software Engineer

Pedal AI — Jul 2025–Dec 2025

- Developed a Python-based backend system for LangGraph AI agents supporting complex, stateful workflows and custom tool integration in chemical applications.
- Built flexible agent nodes and control flows for chemical data pipelines with persistent memory and coordination throughout multi-step processes.
- Worked with backend and product teams to integrate AI agents with molecular prediction engines, providing a consistent API interface and preserved internal state across each run.
- Designed FastAPI connectors across 3 backend layers and 4,000+ lines of code, reducing average prediction latency to under 50 ms while supporting 15,000+ daily API requests and processing 50+ GB of chemical datasets.
- Improved the UI/UX of cheminformatics tools by synchronizing front-end behavior with agent-workflow logic and retrosynthesis route trees; helped evaluate over 100,000 complex molecular predictions with 99.9% system uptime.

Kupcinet-Getz Research Scholar — Computational Biochemical Diffusion

Weizmann Institute of Science, Prof. Semenov — Jun 2025–Aug 2025

- Selected as one of 22 scholars worldwide for the Kupcinet-Getz International School.
- Investigated stochastic differential equations for enzymatic reaction-diffusion systems with Brownian motion, chemical kinetics, spatial heterogeneity, nonlinear biochemical feedback oscillations, molecular self-organization, and chaotic oscillation.
- Developed PINN- and neural-ODE-enhanced stochastic simulation algorithms; implemented custom Euler-Maruyama, Runge-Kutta, and Gillespie SSA solvers.
- Constructed GNN encoders and transformer sequence models with UMAP-driven clustering to extract latent thermal structure from high-dimensional trajectory datasets.

Chemistry and AI Consultant / Scientific Data and Evaluation Specialist

Sepal AI, Mercor — Sept 2024–Feb 2025

- Developed model-training, testing, and evaluation data for LLM workflow applications in graduate-level chemistry reasoning.
- Built grading rubrics and chemical-validity constraints for retrosynthesis, reaction mechanisms, and method-selection tasks.
- Created prompt-engineering, error-analysis, and failure-mode annotation workflows for advanced chemistry reasoning and structured fine-tuning/evaluation data.

Foundation Research Scholar — Computational Organic Chemistry

Lumiere Research Inclusion Foundation — Aug 2023–Feb 2024

- Engineered an automated multi-scale simulation pipeline linking DFT calculations to stochastic kinetic Monte Carlo models.
- Screened 20+ transition states and 500+ reaction trajectories across 5 solvent pathways, reaching a 22% predicted yield optimization for a cytotoxic target.
- Secured a selective full research scholarship and produced a mechanistic manuscript with a Brown University PhD mentor.

Advanced Organic Synthesis Researcher

MIT Chemistry, Prof. Stephen L. Buchwald — Dec 2025–May 2026

- Supported development of CuH-catalyst chemistry for selective asymmetric methylation and alkylation of vinyl boronate esters.
- Used 1H-NMR and chiral-HPLC to connect catalyst structure and activity, expand usable substrate scope, and scale syntheses from 0.1 mmol to multi-gram quantities.

Leadership and Community Involvement

Low Voltage and Software Team Member — Formula SAE Racing Initiative

Columbia University Formula Racing — Jan 2025–May 2025

- Designed PCB systems and embedded software for a Formula SAE electric racing vehicle, focusing on low-voltage microelectronics.
- Collaborated on sensor-network integration and firmware development using Altium Designer and C/C++.

Content Editor and Referee — Columbia Undergraduate Mathematics Journal

Columbia Undergraduate Mathematics Journal — Sept 2024–May 2025

- Critically reviewed senior theses and research papers in mathematics and adjacent fields under graduate mentorship.
- Produced detailed LaTeX referee reports to improve clarity, correctness, structure, and academic rigor.

Dry-Lab Member — MIT BioMakers Lab Initiative

MIT BioMakers — 2026–Present

- Contributing computational and dry-lab support for biology-facing student projects, modeling work, and project infrastructure in MIT's biomaking community.
- Participating in an interdisciplinary ecosystem for student-led biology, engineering, workshops, and community projects.

Undergraduate Advisory / Student Representation

MIT Schwarzman College of Computing Undergraduate Advisory Group · MIT Undergraduate Association — 2026–Present

- Engaging with student-advisory and undergraduate-representation contexts around computing, AI, education, and student experience at MIT.

Olympiad Team Captain and Club President — ACS Chemistry Club and Chemistry Olympiad Team

Üsküdar American Academy — Sept 2020–Jun 2024

- Mentored team members with advanced Olympiad questions for Istanbul, national, and international chemistry competitions; 35 of 50 members placed in top rankings.
- Delegated 15 senior members into organic, inorganic, analytical, and physical chemistry specializations and established peer-mentorship traditions.
- Organized 15 two-hour school-laboratory practical training sessions, including titrations and organic synthesis.

Team Captain — Varsity Male Volleyball Team

Üsküdar American Academy — Sept 2020–Jun 2024

- Conducted the team's offense as primary setter and coordinated weekly training sessions.
- Initiated team-bonding activities and service activities including beach clean-ups.

Honors, Awards, and Recognition

International

- Bronze Medal, 56th International Chemistry Olympiad, Riyadh, Saudi Arabia; ranked 105th among 327 participants, representing Türkiye.
- Bronze Medal, 58th International Mendeleev Chemistry Olympiad, Shenzhen, China; ranked 73rd among 151 participants, representing Türkiye.
- Gold Medal, Lavoisier International Chemistry Olympiad; ranked within the top 5% globally among 500+ participants.
- Certificate of Distinction, University of Waterloo CHEM13 International Chemistry Contest; ranked 2nd among 1,551 participants.

- Certificate of Distinction, Thompson Rivers University Chem12 International Chemistry Contest; ranked 2nd globally.
- AIME Qualification and AMC Hall of Fame acknowledgement; 7th place in Türkiye's country ranking and top 5% AMC 12 score among 150,000+ participants worldwide.
- Certificate of Distinction, Galois International Mathematics Contest; ranked 7th among 3,071 international students and 20th globally among 6,595; medal awarded as top scorer at Üsküdar American Academy.
- Book Prize, Sir Isaac Newton International Physics Contest, University of Waterloo; top 50 globally among 2,000+.

National, Regional, and School-Based

- Silver Medal, TÜBİTAK 31st National Chemistry Olympiad; ranked 3rd among 62 national finalists and 2,500+ students.
- Gold Medal, Istanbul Science Olympiads 2022 in Chemistry; ranked first in Istanbul out of 50 finalists after a 400+ student first stage.
- Gold Award in Physics, 4th Annual KimFiBi Laboratory Competition; first place among 30 high schools.
- Dr. Virginia Canfield Award for Overall Excellence, Üsküdar American Academy, 2022.
- George Ripley Tracy Award for Academic Distinction, Üsküdar American Academy, 2023.
- Graduating Academic Award in Science, Üsküdar American Academy, 2024.

University, Research, and Startup Recognition

- Columbia Science Research Fellow Named Scholar and Likely Letter recipient; awarded full scholarship in recognition of extraordinary scientific talent and accomplishment.
- YC Startup School 2026 Acceptance, associated with Massachusetts Institute of Technology.
- World Science Scholar 2023 Cohort; selected among 52 scholars from 22 countries for exceptional mathematical talent.
- Selected to attend AlgoTrade Hackathon 2026 with free travel and accommodation from 1,000+ applicants across 51 countries and 148 universities.
- Transferred to MIT from Columbia through a 22-from-764, 2.5% acceptance-rate path.

Licenses and Certifications

- Outstanding Success: Assistantships of Augmented Mechanics, Quantum Mechanics, and Augmented Chemistry — Kadir Has University, Prof. A. Nihat Berker, issued Sept 2023.
- Outstanding Success: Phase Transitions and Renormalization Group Theory — Kadir Has University, Prof. A. Nihat Berker, issued Aug 2023.
- Outstanding Success: Quantum Mechanics — Kadir Has University, Prof. A. Nihat Berker, issued Jun 2022.
- Outstanding Success: Augmented Mechanics — Kadir Has University, Prof. A. Nihat Berker, issued Jan 2022.
- Outstanding Success: Augmented Electricity and Magnetism — Kadir Has University, Prof. A. Nihat Berker, issued Aug 2022.

Test Scores

- IBDP: 44/45, November 2023; Higher Level Physics, Chemistry, and Mathematics.
- SAT: 1560; Evidence-Based Reading and Writing 760, Math 800.

Computational and Technical Skillset

- AI/ML: deep learning, machine learning, applied machine learning, reinforcement learning, representation learning, transformers, LLMs, NLP, text mining, pattern recognition, computer vision, dimensionality reduction, automated feature engineering, knowledge engineering, robust optimization, sharpness-aware minimization, fine-tuning, neural networks, DNNs, artificial neural networks, agentic AI development.
- Scientific computing and modeling: Python, C/C++, CUDA, HPC/GPU programming, Linux, Bash, Git, SLURM/PBS/qsub, Conda, distributed training, NumPy, PyTorch, MATLAB, Java, R, LaTeX, parallel computing, system performance, data engineering, data mining, data analytics, predictive modeling, simulation, stochastic differential equations, Monte Carlo simulation.
- Computational chemistry and biophysics: RDKit, CADD, SMILES/SDF/PDB/PDBQT, molecular docking and virtual screening, AutoDock Vina, GNINA CNN scoring, Boltz-2 protein-ligand co-folding, MMGBSA/FEP/free-energy methods, QSAR, RF/XGBoost, ADMET/Rowan, Morgan fingerprints, Tanimoto/PAINS/ESOL filtering, BRICS/generative chemistry, OpenMM, OpenFF, OpenFE, MDTraj, ParmEd, PDBFixer, PySCF, PyMOL, molecular dynamics, molecular modeling, DFT, ab initio methods, synthetic organic chemistry, organic synthesis, theoretical chemistry, quantum chemistry, statistical mechanics, biochemistry, RNA, AlphaFold/IGFold-style metrics.
- Software and data systems: LangGraph, FastAPI, backend web development, software architecture, software documentation, software engineering practices, object-oriented programming, object-oriented languages, full-stack development, UI/UX, user interface design, user experience design, SaaS, PaaS, cloud computing, SQL, Hadoop, data warehousing, data storage technologies, data management, platform architecture.
- Leadership and teaching: assistant teaching, grading, professional mentoring, team leadership, international teams, research skills, scientific writing, academic editing.

Languages

English native; Turkish native; German professional working proficiency; Spanish beginner; Hebrew beginner.

Interests

Philosophy of science, epistemology, logic, metaphysics, psychology, language, history, aesthetics, ethics, politics, power, biopolitics, sociocultural anthropology, Foucauldian studies, love, Judaism, Islam, and critical theories including queer, postmodern, psychoanalytic, post-structuralist, race, and feminist traditions.

Hobbies

Competitive volleyball, chess, poker, personal/political/academic essay editing and writing, figure skating, meditative walking, and labyrinth walking.