Khasan Akhmadiev

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ABOUT ME

✓ Young Scientist specializing in Materials Design through Machine Learning (ML) and Artificial Intelligence (AI), with a focus on data-driven approaches to low-dimensional materials
✓ Research experience in graphene, carbon nanotubes, and twisted bilayer graphene (Twistronics), including applications of AI to study thermodynamic and electronic properties
✓ Active participation in conferences and workshops within the priority fields of Research and Development (R&D)

WORK EXPERIENCE

RUSSIAN QUANTUM CENTER (RQC), QBOARD (SPIN-OFF COMPANY)

INTERNSHIP – 05/2023 – 07/2023

✓ Researched the performance of quantum-inspired optimization algorithms (SIMCIM) for solving NP-hard combinatorial problems, achieving scalable results on Max-Cut, Graph Coloring, Number Partitioning, and Minimum Vertex Cover tasks
✓ Developed Quadratic Unconstrained Binary Optimization (QUBO) models for financial data, enabling investment profit return prediction
✓ Constructed an efficient frontier to analyze the trade-off between expected profit and volatility, contributing to portfolio optimization strategies

EDUCATION AND TRAINING

09/2024 – CURRENT
PHD COMPUTATIONAL MATERIALS SCIENCE Skolkovo Institute of Science and Technology

09/2022 – 09/2024
MS MATERIALS SCIENCE Skolkovo Institute of Science and Technology

09/2018 – 09/2022
BS MATERIALS SCIENCE AND ENGINEERING Tupolev Kazan National Research Technical University

PROJECTS

09/2024 – CURRENT
Investigation of thermodynamical and electronic properties of 2D diamond film using ML

- Generated a dataset of 6000 structural modifications of Diamane using density functional theory (DFT) and ab initio molecular dynamics (AIMD) to enable large-scale training
- Trained a neural network-based interatomic potential to predict atomic interactions with high accuracy
- Studied phonon density of states and band structure of Diamane under rotational misalignment of layers (0–30°), exploring moiré-induced effects
- Calculated thermodynamic properties (entropy, heat capacity, zero-point energy) and benchmarked them against graphene, graphite, and diamond
- Implemented Spectral Energy Density (SED) method for lattice thermal conductivity calculations, developing Python code accelerated with CuPy (GPU) and multiprocessing for high-performance parallel simulations
- Planned extension: electronic property prediction via Deep Learning Tight-Binding (DL-TB) methods for accurate modeling of band structures in rotated 2D systems

02/2024 – 04/2024

Graph Neural Networks for Spatial Time-Series Forecasting (2nd place, ML competition)

- Developed models to forecast cash demand in ATM networks, improving operational planning
- Designed preprocessing pipeline for graph-structured time-series data and tuned model hyperparameters
- Achieved superior predictive accuracy (RMSE, WMAPE) with StemGNN and A3T-GCN, outperforming industry baseline Prophet

11/2023 – 05/2024

Evanescent Wave Fiber Optics Sensor

- Developed data preprocessing and visualization pipeline (Python, SciPy), including interpolation and violin plot analysis for time-resolved evaluation
- Contributed to sensor design and fabrication using D-shaped optical fibers; assembled experimental setup with gas chamber
- Investigated sensing performance toward NO_2 gas under varying humidity conditions and analyzed signal degradation mechanisms
- Conducted experiments with alcohol solutions, estimating sensor response and recovery times for performance benchmarking

Publications

Amirov, R.R., **Akhmadiev, K.**, Gaifutdinov, A.M., Andrianova, K.A., Shmelev, A., Gatiatulin, A.K., Zagidullin, A.A., Milyukov, V.A. and Amirova, L.M., 2023. The interaction of triglycidyl phosphate with europium nitrate and properties of obtained metal-containing polymer. Materials Today Chemistry, 29, p.101

SKILLS

Programming Languages

Python | SQL

Frameworks

Pytorch | Scikit-Learn | Numpy | Pandas | CuPy | Numba | Multiprocessing

Courses

Machine Learning | Experimental Data Processing | Advanced Materials Modelling | Deep Learning | Generative Modelling | Generative AI

Languages

Russian (Native) | English (C1 – Advanced)

CONFERENCES AND SEMINARS

Sino-Russian Conference "Matter and Materials", Skoltech

Modeling the structure and stability of Diamane using machine learning methods

Summer School of Machine Learning SMILES-2025

Summer School Project — Diffusion Language Models for Code Comment Translation

- Developed models to translate code comments, using Hugging Face pretrained models (T5, OPUS) as baselines
- Fine-tuned discrete diffusion model (MLDM) and evaluated outputs using BLEU and BERTScore metrics

NETWORKS AND MEMBERSHIPS

10/2022 – 10/2023 Skolkovo Institute of Science and Technology

Career Center Ambassador