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West Lafayette, IN

Zuhal Cakir

Ph. D. Student

SUMMARY

A passionate Ph.D. student with a strong background in computational chemistry, and cheminformatics. A data-driven analyst with the ability to apply machine learning techniques and leverage algorithms to increase the quality of life.

KEY SKILLS

• Solid understanding of computer representation of reactions & molecular descriptors and experience with large reaction datasets.
• Strong Python programming skills and expertise in machine learning methods/platforms (Scikit-Learn, PyTorch)

TECHNICAL SKILLS

Programming languages: Python(5+ years experience), C/C++, Shell (Bash, Zsh), HTML/CSS, Working knowledge: R, SQL
Tools: PyTorch (+Geometric), Tensorflow, Networkx, XGBoost, Dask, Scikit-Learn, PyData Stack, Pandas
Data Science / Modeling Skills: Graph neural networks, Generative models (VAE), Classification algorithms (XGBoost, SVM), Bayesian optimization / Active learning, Unsupervised Learning (k-means, NMF), Data visualization (matplotlib, seaborn)
Material / Molecular modeling: DFT simulations (VASP, GPAW), Molecular Dynamics (LAMMPS), Pymatgen, Aspen plus
Technologies: High-Performance Computing (CPU/GPU), Git, Adobe Photoshop, Blender, GIMP

EDUCATION

Ph. D. in Chemical Engineering — Aug '20 - Present

Purdue University (Anticipated graduation: June 2025) — West Lafayette, IN

- **Data Science in Chemical Engineering:**
  - Python | Data Analysis Using Scipy and Pandas | Data Standardization and Imputation | Statistics and Optimization
  - Supervised and Unsupervised Learning | Reinforcement Learning | Generative Models | Transfer Learning

B. Sc. in Chemical Engineering — Aug '15 - Jun '20

Bogazici University — Istanbul, Turkey

PROFESSIONAL EXPERIENCE

Graduate Research Assistant — Aug '20 - Present

Purdue University — West Lafayette, IN

Advisor: Prof. Jeffrey Greeley

1. Physics-inspired machine learning model for high-throughput catalyst screening

- Accelerated virtual screening of complex catalyst surface models to investigate complicated reaction dynamics
- Graph Neural Networks to encode complex catalyst surfaces in high entropy alloys

2. Statistical modeling, catalyst active-site engineering

- Built a machine learning model to predict the main features dictating the catalyst activity resulting in an improved understanding of the chemical process

Undergraduate Research Assistant — Mar '19 - Aug '20

Bogazici University — Istanbul, Turkey

Advisor: Dr. Betul Uralcan

Molecular Modelling of carbide-derived carbon-based supercapacitors

- Designed electric double-layer capacitors by using MD simulations(LAMMPS), applied Data Mining and Data Visualization tools to analyze and interpret the electrochemical performance of the battery

Advisor: Prof. Kutlu Ulgen

Genome-scale modeling/Quantitative methods

- Developed constraint-based modeling and biochemical network reconstruction simulations with a python tool, COBRApy

CERTIFICATIONS

- **Machine Learning Certification** | Coursera | May '21 - Jul '21

ADDITIONAL INFORMATION

- **Languages**: English (Fluent) and Turkish (Native) **Interests:** wakeboarding, skiing, swimming, scuba diving, sailing, paragliding