

KUTAY BERK SEZGINEL

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Online version available here: <https://kut.ai/cv/>

PROFESSIONAL EXPERIENCE

Computational Modeling Engineer

Numat Technologies, Inc.

Feb 2023 – present

Remote (US)

- Provided computational modeling support for multidisciplinary projects, guiding experiments through simulations. Worked with experimentalists to elucidate findings and performed screening studies to discover new materials.
- Developed novel methods for materials discovery, quality assessment, data analysis, and predictive modeling and integrated them with a custom Laboratory Information Management System (LIMS).
- Led the computational modeling efforts on collaborative research projects with organizations such as NIST, NSF, IBM, Meta and more. Planned design of experiment (DOE), developed software to run simulation studies on high-performance computing clusters, analyzed and presented outcomes.
- Utilized Machine Learning models to accelerate materials discovery efforts and built predictive models using in-house experimental and simulation data to accurately assess material performance.

Jan 2020 – Feb 2023

Senior Data Scientist

Liaison International

Remote (US)

- Build, validate, and troubleshoot machine learning models using internal tools and metrics and perform individual research on various modeling problems.
- Create product roadmaps to determine and implement specific release features for the data science engine (including unit and integration tests for validation) on a quarterly basis while ensuring compliance with SOC 2 Type 2 certification and integration with CI/CD tools to improve process efficiency and code quality.
- Create and maintain an internal website to document library usage, modeling approaches, research experiments and communicate data science results and insights to team members and customers.
- Periodically review customer data and models to identify significant changes and/or issues in the data or predictions, develop software to automate stringent data checks to identify and address inconsistent data issues and leak variables.

Jan 2019 – May 2019

Computational Engineering Fellow

Numat Technologies, Inc.

Skokie, IL

- Developed a proprietary Python library for computational materials design that integrates various molecular simulations tools with high-performance cloud computing (AWS). Created a workflow to perform reproducible and trackable experiments. Ran a high-throughput screening study and built machine learning models to discover next generation candidate materials.
- Designed and 3D printed custom parts to improve speed and decrease material loss during production. Developed process controllers (hardware and software) with a web interface.

EDUCATION

Doctor of Philosophy in Chemical & Petroleum Engineering

University of Pittsburgh, Swanson School of Engineering

Sep 2015 – Jan 2020

Pittsburgh, PA

- Dissertation Title: "*Computational materials design for molecular machinery: From nanoporous crystals to nanoscale racecars*". PI: Dr. Christopher E. Wilmer

Master of Science in Chemical & Biological Engineering

Koc University, Graduate School of Science and Engineering

Sep 2013 – June 2015

Istanbul, Turkey

- Dissertation Title: “Computational and Experimental Investigation of Methane Adsorption in Pure and Ionic Liquid Modified Metal-Organic Frameworks”

Bachelor of Science in Chemical & Biological Engineering

Koc University, School of Engineering

Sep 2008 – June 2013

Istanbul, Turkey

Energy and Environmental Engineering Track

RESEARCH AND TEACHING EXPERIENCE**Graduate Research Assistant**

Hypothetical Materials Lab, University of Pittsburgh

Sep 2015 – Jan 2020

Pittsburgh, PA

- Developed computational methods for functional materials design including materials such as metal-organic frameworks, supramolecular cages, and artificial molecular machines. Performed data analysis and built ML models using open-source and self-developed Python libraries.
- Organization of the world’s first computational nanocar race: [Formula Nano](http://FormulaNano.com).
- Recreation of the lab website (wilmerlab.com) on GitHub and maintenance as web administrator.

Teaching Assistant and Graduate Mentor

Hypothetical Materials Lab, University of Pittsburgh

Spring 2016 – 2020

Pittsburgh, PA

- Mentored undergraduate and graduate students in data collection and analysis for various projects.
- Guided the students in preparation and presentation of research findings.
- Helped prepare teaching material, graded exams and Teaching assistant for 6 classes

Graduate Research Assistant

Nanomaterials, Energy and Molecular Modelling Research Group &

Sep 2013 – June 2015

Koc University University Tüpras Energy Center (KUTEM)

Istanbul, Turkey

- High-throughput screening of porous materials (MOFs) for gas storage and separation applications using molecular simulations. First lab member to automate in-house computational procedures.
- Post-synthetic modifications of porous materials using ionic liquids to improve gas storage/selectivity performances. Characterization by TGA, XRD, FT-IR, surface area and gas adsorption measurements.
- Instructed weekly lab sessions for teaching Aspen HYSYS software. Prepared and graded quizzes for lab sessions, assigned four design projects and evaluated them, proctored the midterms and finals.

PUBLICATIONS & CONFERENCE PRESENTATIONS

- 11 peer reviewed publications (6 first author and 5 second author)
- 500+ citations
- 12 international conference presentations (in-person, oral)

HONORS & AWARDS (selected)

- Braskem America Inc. Award (outstanding PhD student in Chemical Eng., University of Pittsburgh)
- IBM BlueHack Competition, Second Place (2019)
- Innocentive challenge winner *Chemical Sorbents for Fixed Bed Mercury (Hg^0) Control* (\$5000 prize)
- Full Merit Scholarship – University of Pittsburgh PhD & Koc University, BS and MS

INTERESTS

- Music performance and production, yoga, woodworking, 3D printing, scientific visualization