# KUTAY BERK SEZGINEL

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

## PROFESSIONAL EXPERIENCE

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| ***Computational Modeling Engineer*** | Feb 2023 – present |
| Numat Technologies, Inc. | 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.

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| ***Senior Data Scientist*** | Jan 2020 – Feb 2023 |
| 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.

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| ***Computational Engineering Fellow*** | Jan 2019 – May 2019 |
| Numat Technologies, Inc. | Skokie, IL |

* Developed of 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

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| ***Doctor of Philosophy in Chemical & Petroleum Engineering*** | Sep 2015 – Jan 2020 |
| University of Pittsburgh, Swanson School of Engineering | Pittsburgh, PA |

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

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| ***Master of Science in Chemical & Biological Engineering*** | Sep 2013 – June 2015 |
| Koc University, Graduate School of Science and Engineering | Istanbul, Turkey |

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

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| ***Bachelor of Science in Chemical & Biological Engineering*** | Sep 2008 – June 2013 |
| Koc University, School of Engineering | Istanbul, Turkey |
| *Energy and Environmental Engineering Track* |  |

## RESEARCH AND TEACHING EXPERIENCE

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| ***Graduate Research Assistant*** | Sep 2015 – Jan 2020 |
| Hypothetical Materials Lab, University of Pittsburgh | 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](https://formulanano.com/).
* Recreation of the lab website ([wilmerlab.com](https://kutaybs.com/)) on GitHub and maintenance as web administrator.

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| ***Teaching Assistant and Graduate Mentor*** | Spring 2016 – 2020 |
| Hypothetical Materials Lab, University of Pittsburgh | 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

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| ***Graduate Research Assistant*** | Sep 2013 – June 2015 |
| Nanomaterials, Energy and Molecular Modelling Research Group &  Koc University University Tupras 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 (Hg0) 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