# KUTAY BERK SEZGINEL

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<https://kut.ai> | For interactive version of this resume see <https://kut.ai/cv/>

## PROFESSIONAL EXPERIENCE

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| ***Senior Data Scientist*** | Jan 2020 - present |
| 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 learnings 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*”
* Adviser: 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* |  |

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| ***Erasmus Exchange Program*** | Feb 2012 – Aug 2012 |
| Eindhoven University of Technology, School of Engineering | Eindhoven, The Netherlands |

## RESEARCH AND TEACHING EXPERIENCE

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| ***Graduate Research Assistant*** | Sep 2015 – Jan 2020 |
| Hypothetical Materials Lab, University of Pittsburgh | Pittsburgh, PA |

* Computational method development for functional materials design including materials such as metal-organic frameworks, supramolecular cages, and artificial molecular machines. Performing molecular simulations using high-performance computing and data analysis using available and self-developed Python libraries.
* Organization of 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 three undergraduate and two master 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
* 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.

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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 many in-house computational procedures.
* Investigated the structural and thermodynamic properties of MOFs to understand methane adsorption mechanism and constructed models to predict natural gas storage of MOFs at various conditions.
* 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.

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| ***Visiting Research Assistant*** | Feb 2012 - July 2012 |
| Energy Materials & Devices Group, Eindhoven University of Technology | Eindhoven, Netherlands |

* Designed, fabricated and analyzed enzyme (glucose oxidase) dispersed carbon nanotube electrodes. Measured their glucose oxidation performances using various electrochemical measurements.

## PUBLICATIONS

## 9. [Sezginel, K. B., and Wilmer C. E. Modeling diffusion of nanocars on a Cu (110) surface. *Molecular Systems Design & Engineering*, 5 (2020): 1186-1192.](https://pubs.rsc.org/en/content/articlelanding/2020/me/c9me00171a)

## 8. [Sezginel, K. B., Lee S., Babaei, H. and Wilmer, C. E. Effect of flexibility on thermal transport in breathing porous crystals. *Journal of Physical Chemistry C*, 124 (2020): 18604–18608.](https://pubs.rsc.org/en/content/articlelanding/2020/me/c9me00171a)

## 7. [Chao, Z., Sezginel, K. B., Xu, K., Crouch, G. M., Gray, A. E., Wilmer, C. E., Bohn, P. W., Go, D. B., and Fullerton-Shirey, S. K. Silver Nanofilament Formation Dynamics in a Polymer‐Ionic Liquid Thin Film by Direct Write *Advanced Functional Materials*, 20 (2019): 1-8.](https://onlinelibrary.wiley.com/doi/abs/10.1002/adfm.201907950)

## 6. [Gülsoy, Z., Sezginel, K. B., Uzun, A., Keskin, S. and Yıldırım, R. Analysis of CH4 Uptake over Metal–Organic Frameworks Using Data-Mining Tools. *ACS Combinatorial Science*, 21 (2019): 257-268.](https://pubs.acs.org/doi/abs/10.1021/acscombsci.8b00150)

## 5. [Sezginel, K. B., Asinger, P. A., Babaei, H., and Wilmer, C. E. Thermal transport in interpenetrated metal-organic frameworks. *Chemistry of Materials*, 30 (2018): 2281-2286.](http://pubs.acs.org/doi/abs/10.1021/acs.chemmater.7b05015)

## 4. [Sezginel, K. B., Feng, T. and Wilmer, C. E. Discovery of hypothetical hetero-interpenetrated MOFs with arbitrarily dissimilar topologies and unit cell shapes. *CrystEngComm* 19.31 (2017): 4497-4504.](http://pubs.rsc.org/en/content/articlelanding/2017/ce/c7ce00290d)

## 3. [Sezginel, K. B., Keskin, S. and Uzun, A. Tuning the gas separation performance of CuBTC by ionic liquid incorporation. *Langmuir* 32.4 (2016): 1139-1147.](https://pubs.acs.org/doi/abs/10.1021/acs.langmuir.5b04123)

## 2. [Basdogan, Y., Sezginel, K. B. and Keskin, S. Identifying highly selective metal organic frameworks for CH4/H2 separations using computational tools. *Industrial & Engineering Chemistry Research* 54.34 (2015): 8479-8491.](https://pubs.acs.org/doi/abs/10.1021/acs.iecr.5b01901)

## 1. [Sezginel, K. B., Uzun, A. and Keskin S. Multivariable linear models of structural parameters to predict methane uptake in metal–organic frameworks. *Chemical Engineering Science* 124 (2015): 125-134.](https://www.sciencedirect.com/science/article/pii/S0009250914006022)

## CONFERENCE PRESENTATIONS (ORAL)

## Sezginel, K. B., Nash J. and Wilmer, C.E., "How to Design a Fast Nanocar.", *AIChE Annual Meeting*, Orlando, FL, November 11, 2019.

## Sezginel, K. B., Nash J. and Wilmer, C.E., "Tools for computational design of artificial molecular machines.", *ACS 2019*, Orlando, FL, April 4, 2019.

## Sezginel, K. B., Babaei H. and Wilmer, C.E., "Computational Screening of Thermal Conductivity of MOFs.", *MOF 2018 Young Investigator Symposium*, Rotorua, NZ, Dec. 8, 2018.

## Sezginel, K. B., Asinger P. A., Babaei H. and Wilmer, C.E., "Thermal transport in interpenetrated metal-organic frameworks.", *AIChE Annual Meeting*, Pittsburgh, PA, Oct. 31, 2018.

## Sezginel, K. B. and Wilmer, C.E., "Surface Diffusion of Large Molecules: A Computational Study.", *AIChE Annual Meeting*, Pittsburgh, PA, Oct. 28, 2018.

## Sezginel, K. B. and Wilmer, C.E., "Tools for computational design of artificial molecular machines.", *Avogadro User Group Meeting*, Pittsburgh, PA, August 25, 2018

## Sezginel, K. B., Asinger P. A., Babaei H. and Wilmer, C.E., "Thermal transport in entangled metal-organic frameworks.", *Simulators Meeting*, Midwest Thermodynamics and Statistical Mechanics Meeting, Pittsburgh, PA, June 4, 2018.

## Sezginel, K. B., Asinger P. A., Babaei H. and Wilmer, C.E., "Thermal transport in entangled metal-organic frameworks.", *Simulators Meeting*, Carnegie Mellon University, Pittsburgh, PA, May 22, 2018.

## Sezginel, K. B., Feng T., Wilmer, C.E., “Theoretical Prediction of Interpenetrating Metal-Organic Frameworks”, *AIChE Annual Meeting*, San Francisco, CA, Nov. 15, 2016.

## Sezginel, K. B., Feng T., Wilmer, C.E., “Theoretical Prediction of Interpenetrating Metal-Organic Frameworks”, *Simulators Meeting*, Carnegie Mellon University, Pittsburgh, PA, May 25, 2016.

## Sezginel K. B., Uzun A., Keskin S., “Prediction of CH₄ Storage Performance of Metal-Organic Frameworks”, *AIChE Annual Meeting, Atlanta*, GA, Nov. 17, 2014.

## Sezginel K. B., Uzun A., Keskin S., “Prediction of CH₄ Storage Properties of Metal-Organic Frameworks”, *NanoTR*, Yeditepe University Istanbul, Turkey, June 21, 2014.

**HONORS & AWARDS**

## Braskem America Inc. Award (outstanding PhD student in Chemical Eng., University of Pittsburgh)

## IBM BlueHack Competition, Second Place (2019)

## Molecular Sciences and Software Institute (MolSSI) Fellow (2018 Phase I)

## Startup Blitz Pitch Competition, First Place, University of Pittsburgh ($1500 prize)

## Best Graduate Paper Award (Summer `17), Chemical Engineering Department, University of Pittsburgh

## Foresight Institute 2017 Workshop: *Artificial Intelligence for Molecular Machines*

## 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

## SKILLS

Language**Turkish (Native),** English (Advanced), Dutch (Beginner)

**Software**<https://github.com/kbsezginel>

**Development** Python (Advanced), JavaScript, HTML, Jekyll

**Scientific** HPC, Cloud computing, RASPA, Lammps, Orca, CP2K, Materials Studio, Aspen HYSYS

**Graphics**/Video **Blender, Inkscape, Gimp (Intermediate), Adobe Premiere (Beginner)**

**Audio Ableton, Audacity, Logic Pro,**

**Laboratory** FT-IR, PXRD, High Pressure Volumetric Analyzer, Chemisorption Analyzer, TGA, Glovebox

## PERSONAL

* Interested in electronic and jazz music, for original songs: <https://soundcloud.com/kbs_music>
* Scientific visualization portfolio: <https://kbsezginel.github.io/visualization/portfolio>
* 3-D printing, Rasberry PI, woodworking, running
* Favorite Writers: Ray Kurzweil, Eric Drexler, Franz Kafka

## REFERENCES

**Mark Voortman** (Supervisor at Liaison Internation)

Data Science Architect, Othot Inc.

mvoortman@othot.com

**Christopher E. Wilmer** (Primary Investigator during PhD)

Asst. Professor of Chemical and Petroleum Engineering, University of Pittsburgh

[wilmer@pitt.edu](mailto:wilmer@pitt.edu)

**Christopher Brown** (Research collaborator/employer)

Asst. Professor, School of Health and Rehabilitation Sciences, University of Pittsburgh

cbrown1@pitt.edu