# KUTAY BERK SEZGINEL

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<https://kutaybs.com>

## PROFESSIONAL EXPERIENCE

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| ***Senior Data Scientist*** | Jan 2020 |
| Othot Inc. | Pittsburgh, PA |

* Develop data science and machine learning solutions using Python
* Design, implement and maintain new features in the data science engine for use by the platform
* Automate data science activities and apply best software practices

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

* Development of a proprietary Python library for computational materials design. Automation and simplification of various molecular simulations tools and integration with high-performance cloud computing (AWS). Creating a workflow to perform reproducible and trackable experiments. Using the tools developed, research was performed to discover next generation candidate materials.
* Design and 3D printing of a custom part to improve speed and decrease material loss during production.
* Process controller development (hardware and software) with a web interface.

## EDUCATION

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| ***PhD candidate 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”*
* Advisers: Dr. Seda Keskin & Dr. Alper Uzun

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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 EXPERIENCE

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

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| ***Graduate Research Assistant*** | Sep 2013 – June 2015 |
| Nanomaterials, Energy and Molecular Modelling Research Group, Koc University | 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.

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| ***Graduate Research Assistant*** | Sep 2013 – June 2015 |
| Koc University Tupras Energy Center (KUTEM) | Istanbul, Turkey |

* 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 Research Group, Eindhoven University of Technology | Eindhoven, Netherlands |
| Post-synthetic |  |

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

## PUBLICATIONS

## 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. (2019). Silver Nanofilament Formation Dynamics in a Polymer‐Ionic Liquid Thin Film by Direct Write. *Advanced Functional Materials*

## 6. Gulsoy, Z., Sezginel, K. B., Uzun A., Keskin S., and Yildirim R. (2019). Analysis of CH4 uptake over MOFs using data mining tools. *ACS Combinatorial Science*. (featured on the front cover)

## 5. Sezginel, K. B., Asinger P., Babaei H., and Wilmer C.E. (2018). Thermal transport in interpenetrated metal-organic frameworks. *Chemistry of Materials*. (featured on the front cover)

## 4. Sezginel, K.B., Feng T., Wilmer, C.E. (2017). Discovery of hypothetical hetero-interpenetrated MOFs with arbitrarily dissimilar topologies and unit cell shapes. *CrystEngComm*. (featured on the front cover)

## 3. Sezginel, K. B., Keskin, S., & Uzun, A. (2016). Tuning the gas separation performance of CuBTC by ionic liquid incorporation. *Langmuir*.

## 2. Basdogan, Y., Sezginel, K. B., & Keskin, S. (2015). Identifying highly selective metal organic frameworks for CH4/H2 separations using computational tools. *Industrial & Engineering Chemistry Research*.

## 1. Sezginel, K. B., Uzun, A., & Keskin, S. (2015). Multivariable linear models of structural parameters to predict methane uptake in metal–organic frameworks. *Chemical Engineering Science*.

## 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.

## TEACHING AND MENTORING EXPERIENCE

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| ***Graduate Mentor*** | Spring 2016 – 2020 |
| Hypothetical Materials Lab (WilmerLab) | University of 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.

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| ***Teaching Assistant*** | Spring 2017 |
| ENG 0712 (Honors Engineering Analysis and Computing) | University of Pittsburgh, PA |

* Attended lectures to help students with the assignments and graded assignments.

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| ***Teaching Assistant*** | Fall 2013 & Fall 2014 |
| CHBI 403 (Process and Product Design) | Koc University, Istanbul, Turkey |

* 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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| ***Teaching Assistant*** | Spring 2015 |
| CHBI 491 (Chemical and Biological Engineering Senior Project) | Koc University, Istanbul, Turkey |

* Held weekly meetings with project group members and Prof. Can Erkey to discuss the project, assisted the project group members by providing them supportive articles for their project and giving ideas.

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| ***Teaching Assistant*** | Spring 2014 |
| CHEM 103 (General Chemistry) | Koc University, Istanbul, Turkey |

* Attended weekly lab sessions, graded exams, quizzes, lab reports and proctored the exams.

## HONORS & AWARDS

## Braskem America Inc. Award (outstanding PhD student in Chemical Eng. Department, 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 entitled *Chemical Sorbents for Fixed Bed Mercury (Hg0) Control* ($5000 prize)

## Full Merit Scholarship – University of Pittsburgh PhD & Koc University, BS and MS

## Best Chemical and Biological Engineering Senior Project Award (Biodiesel Production from Algae Oil)

## SKILLS

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

***Software***

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

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

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

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

***Audio* Ableton (Advanced), Audacity (Advanced)**

***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

**Christopher E. Wilmer**

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

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**Christopher Brown**

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

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**Alper Uzun**

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