

# KUTAY BERK SEZGINEL

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## PROFESSIONAL EXPERIENCE

### **Senior Data Scientist**

Othot Inc.

Jan 2020  
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

Jan 2019 – May 2019

### **Computational Engineering Fellow**

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

### **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*”
- Adviser: 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*”
- Advisers: Dr. Seda Keskin & Dr. Alper Uzun

### **Bachelor of Science in Chemical & Biological Engineering**

Koc University, School of Engineering  
*Energy and Environmental Engineering Track*

Sep 2008 – June 2013  
Istanbul, Turkey

### **Erasmus Exchange Program**

Eindhoven University of Technology, School of Engineering

Feb 2012 – Aug 2012  
Eindhoven, The Netherlands

## RESEARCH EXPERIENCE

### **Graduate Research Assistant**

Hypothetical Materials Lab (WilmerLab), University of Pittsburgh

Sep 2015 – Jan 2020  
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](http://wilmerlab.com)) on GitHub and maintenance as web administrator.

**Graduate Research Assistant**

Nanomaterials, Energy and Molecular Modelling Research Group, Koc University

Sep 2013 – June 2015

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.

**Graduate Research Assistant**

Koc University Tupras Energy Center (KUTEM)

Sep 2013 – June 2015

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.

**Visiting Research Assistant**

Energy Materials &amp; Devices Research Group, Eindhoven University of Technology

Feb 2012 - July 2012

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 CH<sub>4</sub> 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 CH<sub>4</sub>/H<sub>2</sub> 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 CH<sub>4</sub> Storage Performance of Metal-Organic Frameworks", *AIChE Annual Meeting*, Atlanta, GA, Nov. 17, **2014**.

**Sezginel K. B.**, Uzun A., Keskin S., "Prediction of CH<sub>4</sub> Storage Properties of Metal-Organic Frameworks", *NanoTR*, Yeditepe University Istanbul, Turkey, June 21, **2014**.

## TEACHING AND MENTORING EXPERIENCE

### **Graduate Mentor**

Hypothetical Materials Lab (WilmerLab)

Spring 2016 – 2020

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.

### **Teaching Assistant**

ENG 0712 (Honors Engineering Analysis and Computing)

Spring 2017

University of Pittsburgh, PA

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

### **Teaching Assistant**

CHBI 403 (Process and Product Design)

Fall 2013 & Fall 2014

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.

### **Teaching Assistant**

CHBI 491 (Chemical and Biological Engineering Senior Project)

Spring 2015

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.

### **Teaching Assistant**

CHEM 103 (General Chemistry)

Spring 2014

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 (Hg<sup>0</sup>) 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

<b>Language</b>	Turkish (Native), English (Advanced), Dutch (Beginner)
<b>Software</b>	
<b>Development</b>	Python (Advanced), JavaScript (Advanced), HTML (Intermediate), Jekyll (Intermediate)
<b>GitHub</b>	<a href="https://github.com/kbsezginel">https://github.com/kbsezginel</a>
<b>Scientific</b>	HPC, Cloud computing, RASPA, Lammmps, Orca, CP2K, Materials Studio, Aspen HYSYS
<b>Graphics/Video</b>	Blender (Advanced), Inkscape (Advanced), Gimp (Intermediate), Adobe Premiere (Beginner)
<b>Audio</b>	Ableton (Advanced), Audacity (Advanced)
<b>Laboratory</b>	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](https://soundcloud.com/kbs_music)
- Scientific visualization portfolio: <https://kbsezginel.github.io/visualization/portfolio>
- 3-D printing, Raspberry 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  
+1 (412) 624-9639, wilmer@pitt.edu

### Christopher Brown

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

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### Alper Uzun

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