KUTAY BERK SEZGINEL

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

PROFESSIONAL EXPERIENCE

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

                                                                                  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   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

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"*

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

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

RESEARCH AND TEACHING EXPERIENCE

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) on GitHub and maintenance as web administrator.

Teaching Assistant and 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.
- 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.

Graduate Research Assistant Sep 2013 – June 2015
Nanomaterials, Energy and Molecular Modelling Research Group, Koc University Istanbul, Turkey
Koc University Tupras Energy Center (KUTEM)
- 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.

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

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.

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.

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.

6. Gülsoy, Z., **Sezginel, K. B.**, Uzun, A., Keskin, S. and Yıldırım, R. Analysis of CH_4 Uptake over Metal–Organic Frameworks Using Data-Mining Tools. *ACS Combinatorial Science*, 21 (2019): 257-268.

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.

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.

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.

2. Basdogan, Y., **Sezginel, K. B.** and Keskin, S. Identifying highly selective metal organic frameworks for CH_4/H_2 separations using computational tools. *Industrial & Engineering Chemistry Research* 54.34 (2015): 8479-8491.

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.

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_4 Storage Performance of Metal-Organic Frameworks", *AIChE Annual Meeting, Atlanta*, GA, Nov. 17, **2014**.

Sezginel K. B., Uzun A., Keskin S., "Prediction of CH_4 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. 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^0) 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	https://github.com/kbsezginel
Development	Python (Advanced), JavaScript (Advanced), HTML (Intermediate), Jekyll (Intermedidate)
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

Mark Voortman (Supervisor at Othot)
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
Christopher Brown (Research collaborator/employer)
Asst. Professor, School of Health and Rehabilitation Sciences, University of Pittsburgh
cbrown1@pitt.edu