

KUTAY BERK SEZGINEL

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<https://kutaybs.com/>

OBJECTIVE

Strong analytical thinker with good problem solving and presentation skills. Seeking to apply a thorough understanding of advanced mathematical concepts and extensive programming experience in the position of a Data Scientist. Currently finishing up PhD in computational materials science and looking to find an innovative and team-oriented workplace.

EDUCATION

PhD candidate in Chemical & Petroleum Engineering Sep 2015 – January 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

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

PROFESSIONAL EXPERIENCE

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.

RESEARCH EXPERIENCE

Graduate Research Assistant Sep 2015 – January 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.

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.

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.

PUBLICATIONS

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)

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)

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)

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

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*.

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)

- American Chemical Society Meeting, Spring 2019 (Orlando, FL)
- American Institute of Chemical Engineers Annual Meeting 2014, 2016, 2018 (USA)
- MOF Conference 2018 (Auckland, New Zealand)
- Simulators Meeting 2016, 2018 (Pittsburgh, USA)
- Midwest Thermodynamics and Statistical Mechanics Conference 2018 (Pittsburgh, USA)
- NanoTR 2014 (Istanbul, Turkey)

HONORS & AWARDS

- Molecular Sciences and Software Institute (MoSSI) 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
- 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)
- Carnegie Library of Pittsburgh STACKS featured musician (<https://stacks.carnegielibrary.org/artists/kbs>)

SKILLS

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

Software

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

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

Scientific HPC, Cloud computing, RASPA, Lammmps, 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://kutaybs.com/visualization/portfolio>
- 3-D printing, microcontrollers, home automation, woodworking, climbing, camping