Hakan Demir, Ph.D.

Assistant Professor

Department of Chemical Engineering

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**PERSONAL**

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| Date of Birth | 30.04.1988 |
| **Place of Birth** | Ankara |

# EDUCATION

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| --- | --- |
| 2011-2016 | Georgia Institute of Technology, Chemical Engineering, Ph.D. |
| 2009-2011 | Middle East Technical University, Chemical Engineering, M.S. |
| 2005-2009 | Middle East Technical University, Chemical Engineering, B.S. |

# ACADEMIC POSITIONS

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| --- | --- |
| **March 2025-present** | Assistant Professor, Department of Chemical Engineering, Atılım University, Turkey |
| **May 2023-present** | Postdoctoral Fellow, Department of Natural and Mathematical Sciences, Özyeğin University, Turkey |
| **Feb 2021-April 2023** | Postdoctoral Research Associate, Department of Chemical & Biological Engineering, Koc University, Turkey |
| **Dec 2018-Jan 2021** | Postdoctoral Fellow, Department of Chemical & Biomolecular Engineering, University of Houston, Houston, TX, USA |
| **May 2016-April 2017, July 2017-December 2018** | Postdoctoral Associate, Department of Chemistry, University of Minnesota, Minneapolis, MN, USA |
| **August 2011-May 2016** | Graduate Research/Teaching Assistant, School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, USA |
| **September 2010-August 2011** | Graduate Research/Teaching Assistant, Department of Chemical Engineering, Middle East Technical University, Ankara, Turkey |

**RESEARCH INTERESTS**

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| 1 | Computational Chemistry |
| **2** | Molecular modeling |
| **3** | Monte Carlo simulations |
| **4** | Molecular Dynamics |
| **5** | Quantum Chemical Calculations |
| **6** | Nanoporous materials |
| **7** | Gas storage and separation |
| **8** | Machine learning |

**PUBLICATIONS**

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| --- | --- |
| 1 | H. Demir, and I. Erucar, “Simulation and Machine Learning-Integrated Investigation of Double-Linker MOFs for the Separation of CF4 from CH4 and N2”, *Industrial & Engineering Chemistry Research*, **2024**, *63*, 12605–12619. |
| **2** | H. Demir, and S. Keskin, “A New Era of Modeling MOF‐Based Membranes: Cooperation of Theory and Data Science”, *Macromolecular Materials and Engineering*, **2024**, 309, 2300225. |
| **3** | H. Demir, H. Daglar, H. C. Gulbalkan, G. O. Aksu, and S. Keskin, “Recent advances in computational modeling of MOFs: From molecular simulations to machine learning”, *Coordination Chemistry Reviews*, **2023**, 484, 215112. |
| **4** | H. Demir, and S. Keskin, “Revealing acetylene separation performances of anion-pillared MOFs by combining molecular simulations and machine learning”, *Chemical Engineering Journal*, **2023**, 464, 142731. |
| **5** | H. Demir, G. O. Aksu, H. C. Gulbalkan, and Seda Keskin, “MOF Membranes for CO2 Capture: Past, Present and Future”, *Carbon Capture Science & Technology*, **2022**, 2, 100026. |
| **6** | H. Demir, and S. Keskin, “Multi-Level Computational Screening of *in Silico* Designed MOFs for Efficient SO2 Capture”, *Journal of Physical Chemistry C*, **2022**, 126, 9875-9888. |
| **7** | H. Demir, and S. Keskin, “Hypothetical yet effective: Computational identification of high-performing MOFs for CO2 capture”, *Computers & Chemical Engineering*, **2022**, 160, 107705. |
| **8** | H. Demir, and S. Keskin, “Computational investigation of multifunctional MOFs for adsorption and membrane-based separation of CF4/CH4, CH4/H2, CH4/N2, and N2/H2 mixtures”, Molecular Systems Design & Engineering, **2022**, 7, 1707-1721. |
| **9** | H. Demir, and S. Keskin, “Computational insights into efficient CO2 and H2S capture through zirconium MOFs”, *Journal of CO2 Utilization*, **2022**, 55, 101811. |
| **10** | Hakan Demir, and S. Keskin, “Zr-MOFs for CF4/CH4, CH4/H2, and CH4/N2 separation: towards the goal of discovering stable and effective adsorbents”, *Molecular Systems Design & Engineering*, **2021**, 6, 627-642. |
| **11** | H. Demir, and L. C. Grabow, “Enhancing Technological Applications through Density Functional Theory Modeling of Nanomaterials”, *ACS Applied Nano Materials*, **2020**, 3, 6127-6130. |
| **12** | H. Demir, C. J. Cramer, and J. I. Siepmann, “Computational screening of metal–organic frameworks for biogas purification”, *Molecular Systems Design & Engineering*, **2019**, 4, 1125-1135. |
| **13** | H. Demir, S. J. Stoneburner, W. Jeong, D. Ray, X. Zhang, O. K. Farha, C. J. Cramer, J. I. Siepmann, and L. Gagliardi, “Metal–Organic Frameworks with Metal–Catecholates for O2/N2 Separation”, *Journal of Physical Chemistry C*, **2019**, 123, 12935-12946. |
| **14** | H. Demir, K. S. Walton, and D. S. Sholl, “Computational Screening of Functionalized UiO-66 Materials for Selective Contaminant Removal from Air”, *Journal of Physical Chemistry C*, **2017**, 121, 20396-20406. |
| **15** | M. A Susner, M. Chyasnavichyus, A. A. Puretzky, Q. He, B. S. Conner, Y. Ren, D. A. Cullen, P. Ganesh, D. Shin, H. Demir, J. W. McMurray, A. Y. Borisevich, P. Maksymovych, and M. A. McGuire, “Cation–Eutectic Transition via Sublattice Melting in CuInP2S6/In4/3P2S6 van der Waals Layered Crystals”,  *ACS Nano*, **2017**, 11, 7060-7073. |
| **16** | D. Yang, M. R. Momeni, H. Demir, D. R. Pahls, M. Rimoldi, T. C. Wang, O. K. Farha, J. T. Hupp, C. J. Cramer, B. C. Gates, and L. Gagliardi, “Computationally Guided Discovery of Metal-Decorated Metal–Organic Frameworks Active for Catalysis”, *Faraday Discussions*, **2017**, 201, 195-206. |
| **17** | T. Chen, X. Lei, H. Demir, C. J. Cramer, L. Gagliardi, and S. J. Guy, “MOF: creating an educational game on nanotechnology through simulation-driven optimization”, *MIG ’16 Proceedings of the 9th International Conference on Motion in Games*, Burlingame, CA, 4-12 October 2016. |
| **18** | M. A. Susner, A. Belianinov, A. Y. Borisevich, Q. He, H. Demir, D. S. Sholl, P. Ganesh, D. L. Abernathy, M. A. McGuire, and P. Maksymovych, “High *Tc* layered ferrielectric crystals by coherent spinodal decomposition”, *ACS Nano*, **2015**, 9, 12365-12373. |
| **19** | H. Demir, J. A. Greathouse, C. L. Staiger, J. J. Perry IV, M. D. Allendorf, and D. S. Sholl, “DFT-based force field development for noble gas adsorption in metal organic frameworks”, *Journal of Materials Chemistry A*, **2015**, 3, 23539–23548. |
| **20** | M. V. Parkes, H. Demir, S. L. Teich-McGoldrick, D. S. Sholl, J. A. Greathouse, and M. D. Allendorf, “Molecular dynamics simulation of framework flexibility effects on noble gas diffusion in HKUST-1 and ZIF-8”, *Microporous and Mesoporous Materials*, **2014**, 194, 190-199. |
| **21** | H. Fang, H. Demir, P. Kamakoti, and D. S. Sholl, “Recent developments in first principles force fields for molecules in nanoporous materials”, *Journal of Materials Chemistry A*, **2014**, 2, 274-291. |

**PROJECTS**

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| --- | --- |
| 1 | TUBITAK 3501 Project, “Developing ionic liquid/metal-organic framework (IL/MOF) composites for effective separation of natural gas and investigating composites’ separation performances using classical molecular simulation and machine learning”, 2024-2026, Principal Investigator |
| **2** | TUBITAK 2218 Project, “Computational design of new generation MOF and MOF-MOF composites to improve energy efficiency of carbon capture technology and development of carbon capture performances thereof via  machine learning models”, 2024-2026, Principal Investigator |
| **3** | Koc University Seed Research Project, “Combatting COVID-19 through metal-organic frameworks (MOFs)”, 2021-2023, Principal Investigator |
| **4** | ERC-2017-Starting Grant, “Computational simulations of MOFs for gas separations”, 2017-2024, Researcher |
| **5** | University of Houston Project, “Computational investigation of metal involving surfaces for methane reactions”, 2018-2021, Researcher |
| **6** | University of Minnesota Project, “Computational investigation of metal-organic frameworks for gas storage/separation and catalysis applications”, 2016-2018, Researcher |
| **7** | Georgia Institute of Technology Project, “Computational exploration of thermodynamic properties of porous and layered materials”, 2011-2016, Researcher |
| **8** | TUBITAK 2228 Project, “Dimethyl ether (DME) synthesis using mesoporous SAPO-34 like catalytic materials”, 2009-2011, Researcher |

# CONFERENCE PRESENTATIONS

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| 1 | Hakan Demir, and Lars C. Grabow, ”Potential benefits of plasma-assisted catalysis on the partial oxidation and dry reforming of methane”, Oral presentation (virtual), ACS Spring 2021 Meeting. |
| 2 | Hakan Demir, Christopher J. Cramer, and Laura Gagliardi, ”A Computational Mechanism Study of Ethylene Dimerization and Hydrogenation on Iridium Loaded NU-1000 and UiO-66”, Oral presentation, AIChE Annual Meeting 2017, Minneapolis, MN. |
| 3 | Hakan Demir, Mohammad R. Momeni, Dale R. Pahls, Laura Gagliardi, and Christopher J. Cramer, ”A Computational Investigation of Ethylene Dimerization and Hydrogenation Mechanisms on Iridium Deposited NU-1000 and UiO-66”, Poster presentation, ICDC All-Hands Meeting 2017, Minneapolis, MN. |
| 4 | Hakan Demir, Krista S. Walton, and David S. Sholl, “Using Computational Modeling to Identify Functionalization Strategies for Selective Contaminant Removal from Ambient Air with UiO-66”, Oral presentation, AIChE Annual Meeting 2014, Atlanta, GA. |
| 5 | Hakan Demir, Jeffery A. Greathouse, and David S. Sholl, “Development and Application of Ab-Initio Based Force Fields for Noble Gas Adsorption in MOFs”, Oral presentation, AIChE Annual Meeting 2014, Atlanta, GA. |

**CITATIONS**

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| Sum of times cited without self-citations (ISI Web of Science): | 714 |
| H-index (ISI Web of Science): | 14 |