Mohammad R. Momeni, Ph.D.

Assistant Professor of Chemistry
University of Missouri–Kansas City (UMKC)
5100 Rockhill Road, Kansas City, MO 64110
Ph: 816-235-2295, Email: mmomenitaheri@umkc.edu
Webpage: https://info.umkc.edu/momenigroup/

EDUCATION

2012–2015	Ph.D. in Theoretical Chemistry, University of Alberta, Edmonton, AB
2006–2011	M.S. in Chemistry, Tarbiat Modares University, Tehran, IR
2002–2006	B.S. in Chemistry, University of Kashan, Kashan, IR

EMPLOYMENT

2022–	Assistant Professor of Chemistry, UMKC
2019–2022	Postdoctoral Research Associate, NJIT
2018–2019	Postdoctoral Research Associate, UC San Diego
2016–2018	Postdoctoral Research Associate, University of Minnesota

RESEARCH SUPPORTS/GRANTS *PI OR CO-PI GRANS (DOE, NSF, UMKC)*

1. *Department of Energy (DOE) BES*, co-PI, $600,000, 2023-2026
2. *National Science Foundation (NSF) CBET*, PI, $120,000, 2023-2026
3. *National Science Foundation (NSF) DMR*, co-PI, $310,000, 2023-2025
4. *Faculty Research Grant-UMKC FFE*, co-PI, $30,000. 02/2023-12/2023

AWARDS & HONORS

- *UMKC Tier 1 Funding for Excellence Award (**2023**)*
- *Mary Louise Imrie Graduate Student Award (**2015**)*
- *Graduate Student Association Professional Development Awards (**2014 & 2015**)*
- *University of Alberta Doctoral Recruitment Scholarship (**2012**)*

CURRENT POSTDOCTORAL SCHOLARS AND PHD STUDENTS

1. Dr. Dil K. Limbu, Postdoc, 03/2023- Email: dil.limbu@umkc.edu
2. Dr. Nathan London, Postdoc, 06/2023- Email: nlondon@umkc.edu
3. Ms. Suchona Akter, PhD student, 06/2023- Email: sad8b@umkc.edu
4. Mr. MD Omar Faruque, PhD student, 06/2023- Email: faruquem@mail.umkc.edu

OPEN-SOURCE SOFTWARE

Momeni, M. R.; Shakib, F. A. *The DL_POLY Quantum Molecular Simulation Package*. Available from: https://github.com/mrmomeni/DL_POLY-Quantum-v1.0.

PEER-REVIEWED BOOK CHAPTER

Downscaling an Open Quantum System: An Atomistic Approach Applied to Photovoltaics, Dell'Angelo, D.; **Momeni, M. R.** Brown, S.E. and Shakib, F.A. (**Green Chemistry and Computational Chemistry: Shared Lessons in Sustainability**, Edited by Liliana Mammino, Pub. Date: November 17, **2021**, Elsevier.)

PEER-REVIEWED PUBLICATIONS (SELECTED, GOOGLE SCHOLAR)

* (corresponding authors) † (Shared first authorship)

1. *Effects of Defects and Presence of Open-Metal Sites on the Structure and Dynamics of Water in Hydrophobic Zeolitic-Imidazolate Frameworks*, Shi, Y.; Limbu, D. K.; Zhang, Z.; **Momeni, M. R.***; Shakib, F. A.* *J. Chem. Inf. Model.* **2023**, *63*, 7097-7106.
2. *In Silico High-Throughput Design and Prediction of Structural and Electronic Properties of Low-Dimensional Metal–Organic Frameworks*, Zhang, Z.; Valente, D.; Shi, Y.; Limbu, D. K.; **Momeni, M. R.***; Shakib, F. A.* *ACS Appl. Mater. Interfaces*, **2023**, *15*, 9494-9507.
3. *Water Induced Structural Transformations in Flexible Two-Dimensional Layered Conductive Metal–Organic Frameworks*, Shi, Y.; **Momeni, M. R.***, Yen-Jui, C.; Limbu, D. K.; Zhang, Z.; Shakib, F. A.***** *Chem. Mater.* **2022**, 34, 7730-7740.
4. *Modeling Energy Transfer and Absorption Spectra in Layered Metal-Organic Frameworks based on a Frenkel-Holstein Hamiltonian*, Dell'Angelo, D.*; **Momeni, M. R.**; Pearson, S.; Shakib, F.A.* *J. Chem. Phys.* **2022**, *156*, 044109 (**Special Issue on "*Transport of Charge and Energy in Low-Dimensional Materials*"**)
5. *Metal–to–Semiconductor Transition in Two-dimensional Metal-Organic Frameworks: An Ab Initio Dynamics Perspective*, Zhang, Z.; Dell'Angelo, D.*; **Momeni, M. R.***; Shi, Y.; Shakib, F. A.* *ACS Appl. Mater. Interfaces*, **2021**, 13, 25270-25279.
6. *Tuning Electronic Properties of Conductive 2D Layered MOFs via Host-Guest Interactions: Dioxygen As An Electroactive Chemical Stimuli*, **Momeni, M. R.***; Zhang, Z.; Dell'Angelo, D.; Shakib, F. A.* *APL Mater.* **2021**, *9*, 051109. (**Special Topic on "*2D Materials Chemistry*", Open Access**)
7. *Deterministic Role of Structural Flexibility on Catalytic Activity of Conductive 2D Layered Metal-Organic Frameworks*, **Momeni, M. R.***; Zhang, Z.; Shakib, F. A.* *Chem. Commun.* **2021**, *57*, 315–318. (**Front Cover**)
8. *Gauging van der Waals Interactions in Aqueous Solutions of 2D MOFs: When Water Likes Organic Linkers More than Open-metal Sites*, **Momeni, M. R.***; Zhang, Z.; Dell'Angelo, D.; Shakib, F. A.* *Phys. Chem. Chem. Phys.* **2021**, *23*, 3135-3143.
9. *Halogen Bonding in UiO-66 Frameworks Promotes Superior Chemical Warfare Agent Simulant Degradation*, Kalaj, M.; **Momeni, M. R.**; Bentz, K. C.; Barcus, K. S.; Palomba, J. M.; Paesani, F.; Cohen, S. M.* *Chem. Commun.* **2019**, 55, 3481-3484.
10. *Computational Screening of Roles of Defects and Metal Substitution on Reactivity of Different Single-vs Double-Node Metal–Organic Frameworks for Sarin Decomposition*, **Momeni, M. R.***; Cramer, C. J. *J. Phys. Chem. C* **2019**, 123, 15157-15165.
11. *Dual Role of Water in Heterogeneous Catalytic Hydrolysis of Sarin by Zirconium-based Metal-organic Frameworks*, **Momeni, M. R.***; Cramer, C. J. *ACS Appl. Mater. Interfaces* **2018**, *10*, 18435-18439.
12. *Structural Characterization of Pristine and Defected* $[Zr_{12}(\mu_3\text{-}O)_8(\mu_3\text{-}OH)_8(\mu_2\text{-}OH)_6]^{18+}$ *Double-Node Metal-organic Framework and Predicted Applications for Single-Site Catalytic Hydrolysis of Sarin*, **Momeni, M. R.***; Cramer, C. J. *Chem. Mater.* **2018**, *30*, 4432-4439.
13. *Density Functional Modeling of Ligand Effects on Electronic Structure and C-H Bond Activation Activity of Copper(III)-Hydroxide Compounds*, Dereli, B.†; **Momeni, M. R.**†; Cramer, C. J.* *Inorg. Chem.* **2018**, 57, 9807-9813.
14. *Tuning the Properties of Metal-Organic Framework Nodes as Supports of Single-Site Iridium Catalysts: Node Modification by Atomic Layer Deposition of Aluminium*, Yang, D.†; **Momeni, M. R.**†; Demir, H.; Pahls, D. R.; Rimoldi, M.; Wang, T. C.; Farha, O. K.; Hupp, J. T.; Cramer C. J.; Gates, B. C.*; Gagliardi, L.* *Faraday Discuss.* **2017**, *201*, 195-206. (**Part of the Themed Collection: New Directions in Porous Crystalline Materials**).
15. *Intramolecular Singlet Fission in Quinoidal Bi- and Tetrathiophenes: A Comparative Study of Low-Lying Excited Electronic States and Potential Energy Surfaces*, **Momeni, M. R.*** *J. Chem. Theory Comput.* **2016**, *12*, 5067-5075.

16. *A Local CC2 and TDA-DFT Double Hybrid Study on BODIPY/aza-BODIPY Dimers As Heavy Atom Free Triplet Photosensitizers for Photodynamic Therapy Applications*, **Momeni, M. R.**; Brown, A.* *J. Phys. Chem. A* **2016**, *120*, 2550-2560.
17. *Toward Unsaturated Stannylenes Y_2Z=Sn: and Related Compounds with Triplet Electronic Ground States*, Bundhun, A.; **Momeni, M. R.**; Shakib, F. A.; Ramasami, P.; Gaspar P. P.; Schaefer III, H. F. *RSC Adv.* **2016**, *6*, 53749-53759.
18. *Why Do TD-DFT Excitation Energies of BODIPY/aza-BODIPY Families Largely Deviate from Experiment? Answers from Electron Correlated and Multi-reference Methods*, **Momeni, M. R.**; Brown, A.* *J. Chem. Theory Comput.* **2015**, *11*, 2619-2632.
19. *Interplay of Donor-acceptor Interactions in Stabilizing Boron Nitride Compounds: Insights from Theory*, **Momeni, M. R.**; Shulman, L.; Rivard, E.; Brown, A.* *Phys. Chem. Chem. Phys.* **2015**, *17*, 16525-16535, (**Open Access**).
20. *Accessing Zinc Monohydride Cations via Coordinative Interactions*, Lummis, P. A.; **Momeni, M. R.**; Lui, M. W.; McDonald, R.; Ferguson, M. J.; Brown, A.; Rivard, E.* *Angew. Chem. Int. Ed.* **2014**, *53*, 9347-9351.
21. *Controlled Growth of Dichlorogermanium Oligomers from Lewis Basic Hosts*, Al-Rafia, S. M. I.; **Momeni, M. R.**; McDonald, R.; Fergsuson, M. J.; Brown, A.; Rivard, E.* *Angew. Chem. Int. Ed.* **2013**, *125*, 6518-6523 **(VIP Article, Inside Front Cover)**.
22. *Carbene-bound Borane and Silane Adducts: A Comprehensive DFT Study on Their Stability and Propensity for Hydride-mediated Ring Expansion*, **Momeni, M. R.**; Rivard, E.; Brown, A.* *Organometallics* **2013**, *32*, 6201-6208.
23. *Stable Complexes of Parent Digermene: An Inorganic Analogue of Ethylene*, Al-Rafia, S. M. I.; **Momeni, M. R.**; Ferguson, M. J.; McDonald, R.; Brown, A.; Rivard, E.* *Organometallics* **2013**, *32*, 6658-6665. (**Invited Article: Special Issue: Applications of Electrophilic Main Group Organometallic Molecules**)
24. *[n]Imperilenes: Stacked [n]Trannulenes Separated by Planar Cycloalkane Rings*, Shakib, F. A.; **Momeni, M. R.**; Wu, J. I.; Schleyer, P. v. R.; Azizi, Z.; Ghambarian M. *Org. Lett*, **2011**, *13*, 3600.
25. *Theoretical Description of Triplet Silylenes Evolved from H_2Si=Si*, **Momeni, M. R.**; Shakib, F. A. *Organometallics*, **2011**, *30*, 5027.
26. *New Generation of Dialkylsilylenes with Stabilities Comparable to Diaminosilylenes: A Theoretical Study*, **Momeni, M. R.**; Shakib, F. A.; Azizi, Z. *J. Phys. Chem. A*, **2011**, *115*, 10550.
27. *Carbenes with Reduced Heteroatom Stabilization: A Computational Approach*, Kassaee, M. Z.; Shakib, F. A.; **Momeni, M. R.**; Ghambarian, M.; Musavi, S. M. *J. Org. Chem.*, **2010**, *75*, 2539.

PRESENTATIONS

1. **Momeni, M. R.** November 30, **2023**, Department of the Physics, Astronomy & Materials Science, Missouri State University, Springfield, MO (Invited Talk).
2. **Momeni**, **M. R.**, October 20, **2023**, ACS Joint Midwest & Great Lakes Regional Meeting, St. Louis, MO (Invited Talk).
3. **Momeni, M. R.** April 29, **2023**, Missouri Inorganic Day **2023** at Missouri S&T, Rolla, MO (Invited Talk)
4. **Momeni, M. R.** *Advanced Materials* Program of the TMS **2023** Annual Meeting, San Diego, CA (Invited Talk)
5. **Momeni, M. R.** Departmental Seminar, Sep **2022**, UMKC (Invited Talk).
6. **Momeni, M. R.** Departmental Seminar, Sep **2022**, KU Lawrence (Invited Talk).
7. **Momeni**, **M. R.** *Path Integral Molecular Dynamics Simulations of the Nanoconfined Water at the Interface with Nanoporous Materials,* Session*: Quantum Dynamics and Light-Matter Interactions*, October 21, **2022**, ACS Northeast Regional Meeting Rochester NY.
8. **Momeni**, **M. R.** *Molecular Level Insights on Nanoporous Materials in Condensed Phases from Atomistic Molecular Dynamics Simulations*, Session: *Computational Methods and Applications*, October 4, **2022**, ACS Midwest Regional Meeting, Iowa City IA.
9. **Momeni**, **M. R.** *Structure-Property Relationships in Multifunctional 2D and 3D Metal-Organic Frameworks in Condensed Phases*, June **2022**, ACS Middle Atlantic Regional Meeting, Trenton, NJ.

10. **Momeni**, **M. R.**; Dell'Angelo, D.; Shakib, F. A. *Modulating Optical Properties of BODIPY Aggregates Encapsulated in Coordination Cages*, April **2021**, ACS Spring Meeting, (Virtual), (**Presider of the session**).
11. **Momeni**, **M. R.** *Temperature and Humidity Triggered Framework Heterogeneity and Disorder and Its Impact on Catalytic Activity of 2D Metal-Organic Frameworks*, November **2020**, MRS Virtual Spring/Fall Meeting.
12. **Momeni**, **M. R.** *Computer Aided Heterogeneous Catalyst Design and Discovery of Single-Atom and Single-Atom Alloyed Transition Metal Catalysts Deposited on Metal-organic Frameworks with Applications in Hydrogen Production from the Shale Gas*, March **2020**, 259th ACS Spring Meeting, Philadelphia, PA.
13. **Momeni**, **M. R.**; Cramer, C. J. *Heterogeneous Catalysis in MOFs: Detoxification of CWAs and Hydrogenative Reduction of CO_2*, October **2017**, Nanoporous Materials Genome Center Phase-II Kick-Off Meeting, University of Minnesota.
14. **Momeni**, **M. R.**; Cramer, C. J. Metal-organic *framework's acid dissociation constants as a robust descriptor of their morphology and reactivity: Applications to hydrolysis of warfare agents*, August **2017**, 254th ACS Fall Meeting, Washington D.C.
15. **Momeni**, **M. R.** *Unravelling Singlet Fission Mechanism in Quinoidal Systems*, August **2017**, 254th ACS Fall Meeting, Washington D.C.
16. **Momeni**, **M. R.** *Dynamically Corrected Methods Can Explain Observed Discrepancies in Singlet Fission Properties of Quinoidal Bi- and Tetrathiophenes*, March **2017**, APS March Meeting, New Orleans, Louisiana.
17. **Momeni**, **M. R.**; Yang, D.; Rimoldi, M.; Wang, T. C.; Farha, O. K.; Hupp, J. T.; Cramer, C. J.; Gates, B. C.; Gagliardi, L. *Tuning the Properties of Metal Organic Framework Nodes as Supports of Single-Site Iridium Catalysts*, October **2016**, Nanoporous Materials Genome Center All-Hands Meeting, The Westin Minneapolis Hotel, Minnesota.
18. **Momeni**, **M. R.**; Brown, A. *Why Do TD-DFT Excitation Energies of BODIPY/Aza-BODIPY Families Largely Deviate from Experiment? Answers from Benchmark of Electron Correlated and Multi-reference Methods*, June **2015**, 98th Canadian Chemistry Conference and Exhibition, Ottawa, Canada.
19. **Momeni**, **M. R.**; Brown, A. *To Branch or Not Branch: A Computational Study on the Carbene Supported Oligogermylenes*, August **2013**, 7th Annual Symposium on Theoretical and Experimental Spectroscopy and Dynamics, Jasper, AB, Canada.

COURSES TAUGHT

UNDERGRADUATE LEVEL COURSES

CHEM 236–Physical Chemistry for Chemical Engineers, 35 enrolments, Fall **2019** (NJIT)
CHEM 235A/339–Physical & Analytical Chemistry Laboratory, 15 enrolments, Fall **2019** (NJIT)
CHEM 125–General Chemistry I, 20 enrolments, Fall **2019** (NJIT)
CHEM 236-001–Physical Chemistry for Chemical Engineers, 25 enrolments, Spring **2020** (NJIT)
CHEM 236-002–Physical Chemistry for Chemical Engineers, 24 enrolments, Spring **2020** (NJIT)
CHEM 126-008–General Chemistry II, 22 enrolments, Spring **2020** (NJIT)
CHEM 126A–General Chemistry Lab II, 14 enrolments, Spring **2020** (NJIT)
CHEM 480–Computer Applications to Chemical Problems, 15 enrolments, Spring **2023** (UMKC)
CHEM 431–Physical Chemistry I, 8 students, Fall **2023** (UMKC)

GRADUATE LEVEL COURSES

CHEM 5580R–Computer Applications to Chemical Problems, 10 enrolments, Spring **2023** (UMKC)

SYNERGISTIC ACTIVITIES

1. **Released Publicly Available & Open Access Software** "DL-*POLY Quantum Molecular Simulation Software Package*" available from: https://github.com/mrmomeni/DL_POLY-Quantum-v1.0.
2. **Panelist and reviewer** for NSF, DOE, and ACS.
3. **Co-organized the Summer School,** *"Computational Chemistry & Molecular Dynamics Summer School"*, July **2022**, NJIT.
4. **Reviewer** for *J. Am. Chem. Soc., Angew. Chem. Int. Ed., Chem. Sci., ACS Cat., J. Cat., J. Comput. Chem., Organometallics, J. Phys. Chem. C, Phys. Chem. Chem. Phys., J. Phys. Org. Chem.* (https://publons.com/researcher/1317696/mohammad-r-momeni/)
5. **Presided the ACS Symposium on Coordination Chemistry**, ACS **2021** Spring Meeting (Virtual).
6. **Served As Judge for the 2019 13th Annual ACS-SA Undergraduate Research Symposium**, UC San Diego, San Diego, California, United States.
7. **Served As Judge for the 2017 Undergraduate Research Symposium**, University of Minnesota, Minneapolis, Minnesota, United States.