# Amir Mirzanejad

https://www.mirzanejad.com

## POSITIONS

**Louisiana State University Shreveport** *August 2025 – Present*

Assistant Professor of Chemistry

**Pennsylvania State University** *September 2022 – June 2025*

Postdoctoral Researcher

## EDUCATION

**University of Nevada, Reno** *August 2017 – August 2022*

*Ph.D. Chemistry*

Supervisor: Dr. Sergey Varganov
Thesis: Quantum Mechanical Study of Spin-Forbidden Reactions in Organometallic Catalysis and Astrochemistry

**Sharif University of Technology** *September 2009 – November 2011*

*M.Sc. Physical Chemistry*

**Urmia University** *September 2005 – May 2009*

*B.Sc. Applied Chemistry*

## RESEARCH

**Louisiana State University Shreveport** *August 2025 –Present*

*Assistant Professor*

- Quantum mechanical and molecular dynamics exploration of chemical and biochemical reactions

**Pennsylvania State University** *September 2022 – June 2025*

*Postdoctoral Research*

- *Ab initio* static and molecular dynamics exploration of ground and excited state potential energy surface of electrocyclic reactions
  - Revealed hidden reaction bifurcations in Cope rearrangements using multi-reference quantum chemistry, enabling accurate product outcome prediction beyond commonly used single-reference DFT.
  - Developed a novel approach that allows ground state formation of photochemical (excited state) electrocyclic products, opening new pathway for synthesis of thermally inaccessible stereoisomers.
  - **Research Awarded DE-SC0025352**

**University of Nevada, Reno** *August 2017 – August 2022*

*Graduate Research*

- Chemical kinetics code development – Funded by NSF CHE-1654547
  - Developed a code in Python/Fortran implementing Phase Space and RRKM chemical rate theories for non-adiabatic barrierless reactions.
- Identification of reaction mechanism for unusually low-temperature C-H bond activation – Funded by ACS PRF-60481-ND6
  - Unveiled the mechanism of a previously unknown Fe(II)-catalyzed C($sp^2$)-H bond activation reactions in THF solvent using DFT ($\omega$B97X-D, B3LYP, MN15-L) and wavefunction (MP2, DLPNO-CCSD(T) and CCSD(T)) methods.
- Electronic structure theory development – Funded by ACS PRF-60481-ND6
  - Developed an atomic model for deriving the Morse interatomic potential function. Introduced a quantum-based framework for estimating empirical parameters in the Morse potential from tabulated data that contributes to the development of reactive force fields and basis sets for electronic structure calculations.
- Mechanistic study of reactions under extreme interstellar condition – Funded by NSF CHE-1654547
  - Identified the 14th member in the $C_2H_5NO$ family of molecules and a new functional group.
  - Revealed spin-forbidden mechanisms using high-level quantum chemistry methods to explain the formation of acetamide and N-methyl-formamide in the interstellar space. Also predicted the formation of acetimidic acid that helps future astronomical observation to reveal this molecule in space.

## PUBLICATIONS

### Peer-Reviewed Journal Papers

1. **A. Mirzanejad**, L. Muechler, "Computational Evidence of a Bifurcation in a Cope Rearrangement Proximate to a Forbidden Electrocyclization" https://doi.org/10.26434/chemrxiv-2025-0xsfn.
2. **A. Mirzanejad**, L. Muechler, "Converting Second-order Saddle Points to Transition States: New principles for the Design of $4\pi$ Photoswitches" *ChemPhysChem* (2024), e202400786.
3. **A. Mirzanejad**, S. A. Varganov, "Two-State Spin-Forbidden Formation of Amide Molecules in the Interstellar Medium" *ACS Earth Space Chem.* (2025) 9, 4, 789–794.
4. **A. Mirzanejad**, S. A. Varganov, "Derivation of Morse Potential" *Mol. Phys.* (2024) e2360542.
5. J. Li, **A. Mirzanejad**, W.-H. Dong, K. Liu, M. Richter, X.-Y, Wang, R. Berger, S. Du, W. Auwärter, J. V. Barth, J. Ma, K. Müllen, A. Narita, X. Feng, J.-T. Sun, L. Muechler, C.-A. Palma "Topological classification of cycloadditions occurring on-surface and in the solid-state" *Communications Chemistry* (2025) 388. (Three first authors contributed equally)
6. I. D. Dergachev, V. D. Dergachev, M. Rooein, **A. Mirzanejad**, S. A. Varganov, "Predicting Kinetics and Dynamics of Spin-Dependent Processes" *Acc. Chem. Res.* 56 (2023) 856-866.
7. **A. Mirzanejad**, S. A. Varganov, "The Role of Intermediate Triplet State in Iron-Catalyzed Multi-State C-H Activation" *Phys. Chem. Chem. Phys.* 24 (2022) 20721-20727.
8. M. Elahifard, M. Sadrian, **A. Mirzanejad***, R. Behjatmanesh-Ardakani, S. Ahmadvand, "Dispersion of Defects in $TiO_2$ Semiconductor: Oxygen Vacancies in the Bulk and Surface of Rutile and Anatase" *Catalysts* 10 (2020) 397.
9. S. Ahmadvand, M. Elahifard, M. Jabbarzadeh, **A. Mirzanejad***, et al. "Bacteriostatic Effects of Apatite-Covered Ag/AgBr/$TiO_2$ Nanocomposite in the Dark: Anomaly in Bacterial Motility" *J. Phys. Chem. B* 123 (2019), 787-791.
10. M. Elahifard, S. Ahmadvand, **A. Mirzanejad***, "Effects of Ni-doping on the Photo-catalytic Activity of $TiO_2$ Anatase and Rutile: Simulation and Experiment" *Mater. Sci. Semicond. Process.* 84 (2018) 10-16.
11. **A. Mirzanejad**, "Thermal Chemistry of 2-Halo-1-propanols on Ni(111) and Cu(111) Surfaces: A UBI-QEP Energetic Modeling" *Appl. Surf. Sci.* 359 (2015) 576-588.

## UNDER REVIEW PAPERS

1. Z. Xie, **A. Mirzanejad**, L. Muechler "Topological Transitions in Orbital-Symmetry-Controlled Chemical Reactions" https://doi.org/10.48550/arXiv.2506.18984

## TEACHING

### Textbook Authorship

- "Fundamentals of Physical Chemistry", Author (in Persian), Urmia University.
  - A concise and comprehensive textbook covering all undergraduate physical chemistry courses spanning essential concepts in thermodynamics, phase equilibrium, electrochemistry, chemical kinetics, quantum mechanics, and molecular spectroscopy.

**Louisiana State University Shreveport** *August 2025 - Present*

- Instructor: General and Physical Chemistry
- Instructor: General and Physical Chemistry Lab

**Pennsylvania State University** *March 2023, April 2024*

- Guest Instructor: PhD Quantum Chemistry
  - Geometry Optimization Techniques
  - Basis Sets

*Indicates equal contribution of all authors.

**University of Nevada, Reno** *August 2017 – May 2019*

- Teaching Assistant: General Chemistry Labs 121 and 122
  - Led two semiweekly lab-lecture sections (4-hours each) and held weekly office hours (2-hours); created pre-lab quizzes and lab finals; graded lab assignments and pre-lab quizzes and finals

**Urmia University** *September 2007 – June 2008*

- Teaching Assistant: Physical Chemistry and Analytical Chemistry
  - Led weekly homework assignments review class (2-hours) and created homework questions

## SKILLS

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|---|---|
| Programming: | Python, Fortran |
| Quantum Software & Tools: | Gaussian, GAMESS, Orca, Q-Chem, Molpro, Multiwfn, Multiwell |

## AWARDS & HONORS

- PCCP HOT Article, Journal of Physical Chemistry Chemical Physics, 2022
- GSA Research, Travel and Materials Grant Award, University of Nevada, Reno, Fall 2021
- Hyung Kyu Shin Graduate Scholarship, Chemistry Department, University of Nevada, Reno, 2021
- 3rd Place, The Bay Area Theoretical Chemistry Lightning Talk Competition, Stanford University, 2021
- American Chemical Society paper of the day, Editors' first choice from the entire ACS portfolio, 2019
- Gene and Carla LeMay Scholarship, Chemistry Department, University of Nevada, Reno, 2018

## PRESENTATIONS

1. **A. Mirzanejad**, L. Muechler, "**Oral:** Multi-Reference Approaches Unveil Electrocyclization Bifurcations in Cope Rearrangements" *ACS Spring National Meeting*, New Orleans, 17 - 21 March 2024.
2. **A. Mirzanejad**, C. Daggett, Z. Xie, L. Muechler "**Poster:** Topological Classification of Chemical Reactions: A New Tool to Understand and Manipulate Chemical Reactivity" *Materials Day 2023*, State College, 26 - 27 October 2023.
3. **A. Mirzanejad**, L. Muechler, "**Poster:** Molecular Geometry, Not Orbital Overlap Determines Stereochemistry of Electrocyclic Reactions" *Physical Organic Chemistry Gordon Research Conference*, Holderness, June 25 - 30, 2023.
4. **A. Mirzanejad**, S. A. Varganov, "**Poster:** Multi-State Reactivity in Iron-Activated C–H Bond" *American Conference on Theoretical Chemistry (ACTC)*, Palisades Tahoe, July 25 - 28, 2022.
5. **A. Mirzanejad**, S. A. Varganov, "**Oral:** Iron-Catalyzed Multi-State Activation of C($sp^2$)–H Bond" *ACS Spring 2022 National Meeting*, San Diego, March 20 - 24, 2022.
6. D. S. Kaliakin, **A. Mirzanejad**, A. J. Pohlman, S. M. Casey, S. A. Varganov, "**Oral:** Role of Electron Spin in Catalytic Reaction Mechanisms" *Synergies between Theory, Experiment and Data Science towards Clean Energy*, 2020.
7. **A. Mirzanejad**, S. Ahmadvand, S. A. Varganov, "**Poster:** Spin-Forbidden Formation of Amide Molecules in the Interstellar Medium" *AbGradCon* 2019, Salt Lake City, July 22-26, 2019.
8. **A. Mirzanejad**, S. Ahmadvand, S. A. Varganov, "**Poster:** Computational Modeling of $C_2H_5NO$ Isomers Formation in the Interstellar Medium" *AbGradCon* 2018, Atlanta, June 04 - 08, 2018.