

Room 268, Chemistry Building, University of North Texas • Email: ahmadnajafian@my.unt.edu

Google scholar profile link:

<https://scholar.google.com/citations?user=QD7nXgcAAAAJ&hl=en>

Education

- ❖ **PhD Candidate**, Research Assistant in the Cundari Research Lab, Inorganic Chemistry, University of North Texas, Denton, TX (Fall 2016-present)
Advisor: Prof. Thomas R. Cundari
- ❖ **Master of Science**, Inorganic Chemistry, Iran University of Science and Technology, Tehran, Iran (Sep 2010-2012)
- ❖ **Bachelor of Science**, Applied Chemistry, Bu-Ali Sina University, Hamedan, Iran (2004-2009)

Research Experiences

Cundari Lab (Ph.D.)

University of North Texas, Denton, TX

Inorganic Chemistry

- ✓ Modeling and DFT calculations of organometallic compounds and transition metal catalysts
- ✓ DFT calculations of C-H activation of methane by 3d-metal methoxide catalysts
- ✓ Acetylene hydration by bio-inspired catalyst models that mimic acetylene hydratase enzyme
- ✓ Metalloenzymes, Drug Design, Protein Modeling, Molecular Dynamics

Rahimi lab (M.Sc.):

Iran University of Science & Technology, Tehran, Iran

Inorganic Chemistry

- ✓ Synthesis of heterogeneous catalysts: porphyrins, semiconductors (TiO₂) and porous materials (SBA-15 & SBA-16)
- ✓ Oxidation alkenes, degradation of organic pollutants and removal of heavy metals by heterogeneous catalysts

Research Publications:

1. **A. Najafian** and T. R. Cundari, "C-H Activation of Methane by Nickel-Methoxide Complexes: A DFT study", *Organometallics* **2018**, 37, 3111-3121.
2. **A. Najafian** and T. R. Cundari, "Computational Study of Acetylene Hydration by Bio-inspired Group Six Catalyst Models", *Polyhedron*, **2018**, <https://doi.org/10.1016/j.poly.2018.07.044>. (invited, Bill Jones 65th Birthday Special Issue)
3. **A. Najafian** and T. R. Cundari, "Methane C-H Activation via 3d Metal Methoxide Complexes with Potentially Redox-Noninnocent Pincer Ligands: A Density Functional Theory Study", *Inorg. Chem.*, **2017**, 56, 12282-12290.
4. **A. Najafian**, R. Rahimi, S. Zargari, M. Mahjoub-Moghaddas and A. Nazemi, "Synthesis and photocatalytic activity of V-doped mesoporous TiO₂ photosensitized with porphyrin supported by SBA-15", *Res. Chem. Intermed.*, **2016**, 42, 3441.
5. **A. Najafian**, M. Rabbani, R. Rahimi, M. Deilamkamar and A. Maleki, "Synthesis and characterization of copper porphyrin into SBA-16 through "ship in a bottle" method: A catalyst for photo oxidation reaction under visible light", *Solid State Sci.*, **2015**, 46, 7.
6. A. Nazemi, **A. Najafian**, S. A. S. Sadjadi, "Aluminum oxide nanowires synthesis from high purity aluminum films via two-step anodization", *Superlattices Microstruct.*, **2015** 81, 1-6

Conferences and Presentations:

1. **Ahmad Najafian**, Thomas R. Cundari. "Impact of metal identity and supporting ligand on acetylene hydration by group six catalyst models" Oral presentation at ACS National Meeting, Boston, Massachusetts (Aug 2018).
2. **Ahmad Najafian**, Thomas R. Cundari. "Methane-to-Methanol Conversion by (L_n)Nickel-Methoxide complexes: Effect of Supporting Ligand" Poster at F.G.A. Stone Symposium, Baylor, Texas (May 2018).
3. **Ahmad Najafian**, Thomas R. Cundari. "DFT study of methane C-H activation via 3D metal-methoxide complexes with potentially redox non-innocent pincer ligands" Oral Presentation at ACS Southwest Regional Meeting, Lubbock, Texas (Nov 2017).
4. **Ahmad Najafian**, Thomas R. Cundari. "DFT Study of Methane Activation by 3d Metal Alkoxides". Oral Presentation at ACS Meeting in Miniature, Fort Worth, Texas (March 2017).
5. Rahmatollah Rahimi, **Ahmad Najafian**, Mahboubeh Rabbani, Mehdi Deilamkamar, Ali Maleki; " Synthesis of Copper Porphyrin into SBA-16 Walls as Catalyst for Oxidation Reaction"; 16th International Electronic Conference on Synthetic Organic Chemistry, University of Santiago de Compostela, Spain 2012.
6. Rahmatollah Rahimi, **Ahmad Najafian**, Mehdi Deilamkamar, Ali Maleki, Mahboubeh Rabbani, Samaneh Safaloumoghaddam, "Investigation on Photocatalytic Activity of Porphyrin into Mesoporous Silica as Biomimetic Heterogeneous Catalyst for Degradation of Azo Dyes"; The 3th Iran International Zeolite Conference, Arak, Iran, 6-7 June, 2012.
7. Sina Golafshan, Beheshteh Sohrabi*, **Ahmad Najafian**, " The investigation of surfactants detergency in presence extracted nanostructures from Alliaceae plants", Proceedings of the 4th International Conference on Nanostructures (ICNS4), Kish Island, Iran, 12-14 March, 2012.
8. Sina Golafshan, Beheshteh Sohrabi*, **Ahmad Najafian**, Mohammad Javade Malayeri " The investigation of surface activity behavior and physico-chemical extracted surfactants detergents from Alliaceae plants", 3rd Surfactant & Detergent Technology Conference, Tehran, Iran, 10-11 Oct 2012.
9. Rahmatollah Rahimi*, Mehdi Deilamkamar, **Ahmad Najafian**, Ali Maleki, Mahboubeh Rabbani, "Removal of Heavy Metal from Aqueous Solution by tetrakis(4-carboxyphenyl) Porphyrin-Functionalized SBA-15 Mesoporous Silica", The 3rd Iran International Zeolite Conference, Arak, Iran, 6-7 June, 2012.
10. Samaneh Safalou Moghaddam, Rahmatollah Rahimi, Mahboubeh Rabbani, **Ahmad Najafian**, "Photocatalytic degradation of methylene blue with porphyrin-sensitized N, S-codoped TiO₂ under visible light"; The 3rd Iran International Zeolite Conference, Arak, Iran, 6-7 June, 2012.

Teaching and Work Experiences

- Collaboration with Reata Pharmaceuticals (<https://www.reatapharma.com/>) on drug design and protein modeling (Oct 2017 – present)
- Research Assistant in Dr. Thomas Cundari's Research Group, University of North Texas Chemistry Department (May 2017 – present)
- Teaching Assistant, University of North Texas, Chemistry Department (Sep 2016 – May 2017)
- Research Assistant in Dr. Rahimi's Research Group, Iran University of Science and Technology, Chemistry Department (Sep 2014 – April 2016)
- Dr. Abidi Pharmaceuticals company in quality control (QC) department (July 2013 – Jun 2014)
- Teaching Assistant (TA) for the course "General Chemistry", Iran University of Science and Technology, Tehran, Iran (Fall 2011)

Membership

- Member of American Chemical Society (ACS)