

# Ahmad Najafian

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## Education

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- **Ph.D. candidate**, in Inorganic Chemistry, University of North Texas (Sept. 2016 - present)  
Advisor: Prof. Thomas R. Cundari
- **Master of Science**, in Inorganic Chemistry, Iran University of Science & Technology (Sept. 2010 - 2012)
- **Bachelor of Science**, in Applied Chemistry, Bu-Ali Sina University, Hamedan, Iran (Sept. 2004 - 2009)

## Research Experiences

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- **Cundari Lab (Ph.D.)**  
University of North Texas, Denton, TX

### Computational Inorganic Chemistry

- ✓ Modeling and Quantum Mechanics (DFT) calculations of organometallic catalysts
- ✓ C–H and N–H bond activation of small molecules by transition metal complexes for renewable energies
- ✓ Mechanistic study of metalloenzymes active sites and their reactions
- ✓ Drug Design, Protein Modeling, Molecular Dynamics, QM/MM

- **Rahimi lab (M.Sc.):**  
Iran University of Science & Technology, Tehran, Iran

### Synthetic Inorganic Chemistry

- ✓ Synthesis of heterogeneous catalysts, porphyrins, semiconductors (TiO<sub>2</sub>) and porous materials (SBA-15 & SBA-16)
- ✓ Oxidation alkenes, degradation of organic pollutants and removal of heavy metals by heterogeneous catalysts

## Peer-Reviewed Publications

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1. **Ahmad Najafian** and Thomas R. Cundari, "DFT Modeling of the Methane-to-Methanol Conversion via Earth-Abundant Late 3d Bimetallic Complexes" *In progress*
2. **Ahmad Najafian** and Thomas R. Cundari, "Effect of S-Block Metal Ion on Redox Properties of Mn(V) Salen-Crown Ether Complexes: Methane Activation" *Inorg. Chem.* **Submitted** (06/07/2019)
3. **Ahmad Najafian** and Thomas R. Cundari, "Computational Mechanistic Study of Electro-oxidation of Ammonia to N<sub>2</sub> by Homogenous Ruthenium and Iron Complexes" *J. Phys. Chem. A* **Submitted** (06/20/2019)
4. **Ahmad Najafian** and Thomas R. Cundari, "C-H Activation of Methane by Nickel-Methoxide Complexes: A DFT study" *Organometallics* **2018**, 37, 3111-3121. [[DOI](#)]
5. **Ahmad Najafian** and Thomas R. Cundari, "Computational Study of Acetylene Hydration by Bio-inspired Group Six Catalyst Models" *Polyhedron*, **2018**, 154, 114-122. (Invited, Bill Jones 65<sup>th</sup> Birthday Special Issue) [[DOI](#)]
6. **Ahmad Najafian** and Thomas 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. [[DOI](#)]
7. **Ahmad Najafian**, Rahmatollah Rahimi, Solmaz Zargari, Masoumeh Mahjoub-Moghaddas and Azadeh Nazemi, "Synthesis and Photocatalytic Activity of V-doped Mesoporous TiO<sub>2</sub> Photosensitized with Porphyrin Supported by SBA-15" *Res. Chem. Intermed.*, **2016**, 42, 3441-3458. [[DOI](#)]
8. **Ahmad Najafian**, Mahboubeh Rabbani, Rahmatollah Rahimi, Mehdi Deilamkamar and Ali 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, 7-13. [[DOI](#)]
9. Azadeh Nazemi, **Ahmad Najafian**, Seyed. A. S. Sadjadi, "Aluminum Oxide Nanowires Synthesis from High Purity Aluminum Films via Two-Step Anodization" *Superlattices Microstruct.* **2015**, 81, 1-6. [[DOI](#)]

## Highlighted Presentations

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1. **Ahmad Najafian**, Thomas R. Cundari. "DFT modeling of the complete catalytic cycle of methane-to-methanol via Earth-abundant late 3d bimetallic complexes" **Poster** at ACS National Meeting, Orlando, FL (April 2019).
2. **Ahmad Najafian**, Thomas R. Cundari. "Impact of metal identity and supporting ligand on acetylene hydration by group six catalyst models" **Talk** at ACS National Meeting, Boston, MA (Aug. 2018).
3. **Ahmad Najafian**, Thomas R. Cundari. "Methane-to-Methanol Conversion by (L<sub>n</sub>)Nickel-Methoxide complexes: Effect of Supporting Ligand" **Poster** at F.G.A. Stone Symposium, Baylor, TX (May 2018).
4. **Ahmad Najafian**, Thomas R. Cundari. "DFT study of methane C-H activation via 3D metal-methoxide complexes with potentially redox non-innocent pincer ligands" **Talk** at ACS Southwest Regional Meeting, Lubbock, TX (Nov 2017).
5. **Ahmad Najafian**, Thomas R. Cundari. "DFT Study of Methane Activation by 3d Metal Alkoxides" **Talk** at ACS Meeting in Miniature, Fort Worth, TX (March 2017).
6. Rahmatollah Rahimi, **Ahmad Najafian**, Mahboubeh Rabbani, Mehdi Deilamkamar, Ali Maleki; "Synthesis of Copper Porphyrin into SBA-16 Walls as Catalyst for Oxidation Reaction" 16<sup>th</sup> International Electronic Conference on Synthetic Organic Chemistry, Spain 2012.
7. 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" **Talk** at The 3th Iran International Zeolite Conference, Arak, Iran (June 2012).
8. Sina Golafshan, Beheshteh Sohrabi\*, **Ahmad Najafian**, "Investigation on surfactants detergency in presence extracted nanostructures from Alliaceae plants" **Poster** at Proceedings of the 4th International Conference on Nanostructures (ICNS4), Kish Island, Iran (March 2012).
9. Sina Golafshan, Beheshteh Sohrabi\*, **Ahmad Najafian**, Mohammad Javad Malayeri "Investigation on surface activity behavior and physico-chemical extracted surfactants detergents from Alliaceae plants" **Poster** at 3rd Surfactant & Detergent Technology Conference, Tehran, Iran (Oct. 2012).
10. 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" **Poster** at The 3rd Iran International Zeolite Conference, Arak, Iran (June 2012).

### Teaching and Work Experiences

- **Researcher**, Collaboration with Reata Pharmaceuticals ([Website](#)) on drug design and protein modeling (Nov. 2017 - present)
- **Graduate Research Assistant**, in Dr. Thomas Cundari's Research Group, University of North Texas, Chemistry Department (June 2017 - present)
- **Teaching Assistant**, University of North Texas, Chemistry Department (Aug. 2016 - May 2017)
- **Research Assistant**, in Dr. Rahimi's Research Group, Iran University of Science and Technology, Chemistry Department (Sept. 2014 - April 2016)
- **Quality Control Chemist**, at ABIDI Pharmaceutical Company (July 2013 - Jun 2014)
- **Teaching Assistant**, for General Chemistry, Iran University of Science & Technology, Tehran, Iran (Fall 2011)

### Computer Skills

✓ CCDC	✓ Avogadro	✓ ChemCraft	✓ ChemDraw	✓ Gaussian	✓ GaussView
✓ MOE	✓ Chimera	✓ VMD	✓ Python	✓ Linux	

### References

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