Bohak Yoon, Ph.D.

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Education

The University of Texas at Austin, Austin, TX — *2022*
Ph.D. in Chemical Engineering, *Dissertation Fellow*

Lehigh University, Bethlehem, PA — *2016*
B.S. in Chemical Engineering, *Summa Cum Laude*

Professional Appointments

Baylor University, Waco, TX — *Jan 2025 - Present*
Assistant Professor, Department of Chemistry and Biochemistry,
Materials Science and Engineering Program

The University of Chicago, Chicago, IL — *Jul 2022 - Dec 2024*
Postdoctoral Fellow, The Chicago Center for Theoretical Chemistry, Department of Chemistry, James Franck Institute, and Institute for Biophysical Dynamics
Advisor: Dr. Gregory A. Voth

The University of Texas at Austin, Austin, TX — *Sep 2017 - Jun 2022*
Graduate Research Assistant, Department of Chemical Engineering
Advisor: Dr. Gyeong S. Hwang

Lehigh University, Bethlehem, PA — *Jul 2014 - Jun 2016*
Undergraduate Research/Teaching Assistant, Department of Chemical Engineering
Advisors: Dr. Steven McIntosh and Dr. Mark A. Snyder

Publications

Published Peer-Reviewed Journal Articles: (12 first/co-first author & 2 co-author)
[# denotes equal contribution]

14. **Yoon, B.**; Chen, S.; Voth, G. A. "On the Influence of Amino Acid Ionic Liquid Anions on CO2 Capture." *Journal of the American Chemical Society* **2024**, *146*, 1612-1618. DOI: 10.1021/jacs.3c11808
13. Song, Y. I.#; **Yoon, B.#**; Lee, C.; Kim, D.; Han, M. H.; Han, H.; Lee, W. H.; Won, D. H.; Kim, J. K.; Jeon, H. S.; Koh, J. H. "Impact of Side Chains in 1-n-Alkylimidazolium Ionomers on Cu-Catalyzed Electrochemical CO2 Reduction." *Advanced Science* **2024**, *Accepted.* DOI: 10.1002/advs.202406281
12. **Yoon, B.**; Voth, G. A. "Elucidating Molecular Mechanisms of CO2 Capture by Amino Acid Ionic Liquids." *Journal of the American Chemical Society* **2023**, *145*, 15663-15667. DOI: 10.1021/jacs.3c03613
11. Luo, Q.; Ouyang, Y.; Hong, S.; Wang, N.; Li, Y.; Gao, H.; Hwang, G. S.; **Yoon, B.**; Sema, T.; Tontiwachwuthikul, P.; Luo, P.; Saiwan, C.; Liang, Z. "Combined Experimental and Computational Study on the Effect of Solvent Structure on Developing CO2 Biphasic Absorbents." *Separation and Purification Technology* **2023**, *308*, 122856. DOI: 10.1016/j.seppur.2022.122856
10. **Yoon, B.**; Calabro, D. C.; Saunders, L.; Raman, S.; Hwang, G. S. "Probing Strong Steric Hindrance Effects in Aqueous Alkanolamines for CO2 Capture from First Principles." *Journal of Environmental Chemical Engineering* **2022**, *10*, 108987. DOI: 10.1016/j.jece.2022.108987
9. Luo, Q.; Gao, H.; Wang, N.; Li, Y.; Hong, S.; Hwang, G. S.; **Yoon, B.**; Liang, Z. "Development of A Monoethanolamine/n-Butanol Biphasic Solution with Tunable Phase Separation for CO2 Absorption via Combined Experimental and Computational Study: Role of Solvation Environment, Phase Separation Mechanism." *Separation and Purification Technology* **2022**, *301*, 121861. DOI: 10.1016/j.seppur.2022.121861

8. **Yoon, B.**; Hwang, G. S. "Intriguing Thermal Degradation Behavior of Aqueous Piperazine for Carbon Dioxide Capture: A First-Principles Assessment." *ACS Sustainable Chemistry & Engineering* **2022**, *10*, 9584-9590. DOI: 10.1021/acssuschemeng.2c02502

7. Luo, Q.#; **Yoon, B.**#; Gao, H.; Lv, J.; Hwang, G. S.; Xiao, M.; Liang, Z. "Combined Experimental and Computational Study on the Promising Monoethanolamine+2-(Ethylamino)ethanol+Sulfolane Biphasic Aqueous Solution for CO2 Absorption." *Chemical Engineering Journal* **2022**, *49*, 136674. DOI: 10.1016/j.cej.2022.136674

6. Luo, Q.#; Dong. R#; **Yoon, B.**#; Gao, H.; Chen, M.; Hwang, G. S.; Liang, Z. "Experimental/Computational Study of Steric Hindrance Effects on CO2 Absorption in (Non)Aqueous Amine Solutions." *AIChE Journal* **2022**, e17701. DOI: 10.1002/aic.17701

5. **Yoon, B.**; Hwang, G. S. "Facile Carbamic Acid Intermediate Formation in Aqueous Monoethanolamine and its Vital Role in CO2 Capture Processes." *Industrial & Engineering Chemistry Research* **2022**, *61*, 4475-4479. DOI: 10.1021/acs.iecr.1c04987

4. **Yoon, B.**; Hwang, G. S. "First-Principles Assessment of Anomalous Thermal Degradation of Aqueous 2-Amino-2-methyl-1-propanol for CO2 Capture." *Energy & Fuels* **2021**, *35*, 16705-16712. DOI: 10.1021/acs.energyfuels.1c02361

3. **Yoon, B.**; Hwang, G. S. "Anomalous Facile Carbamate Formation at High Stripping Temperatures from Carbon Dioxide Reaction with 2-Amino-2-methyl-1-propanol in Aqueous Solution." *ACS Sustainable Chemistry & Engineering* **2020**, *8*, 18671-18677. DOI: 10.1021/acssuschemeng.0c07203

2. **Yoon, B.**; Hwang, G. S. "On the Mechanism of Predominant Urea Formation from Thermal Degradation of CO2-Loaded Aqueous Ethylenediamine." *Physical Chemistry Chemical Physics* **2020**, *22*, 17336-17343. DOI: 10.1039/D0CP02178D

1. **Yoon, B.**; Stowe, H. M.; Hwang, G. S. "Molecular Mechanisms for Thermal Degradation of CO2-Loaded Aqueous Monoethanolamine: A First-Principles Study." *Physical Chemistry Chemical Physics* **2019**, *21*, 22132-22139. DOI: 10.1039/C9CP04518J

Submitted/In-preparation: (1 submitted & 4 in-preparation)

5. Zhang, W.; Fang, S.; Su, H.; Hao, W.; **Yoon, B.**; Hwang, G. S.; Cheng, C.; Zhu, Y.; Hu, Y. H. "Water-Superstructured Solid Fuel Cells." *Under review.* arXiv: 2110.15126

4. Chen, S.; Yang, C.; **Yoon, B.**; Wu, J.; Voth, G. A. "Capturing the Polarization Effect of Choline-Based Amino Acid Ionic Liquids in Molecular Dynamics Simulations." *In-preparation.*

3. **Yoon, B.**; Patel, D.; Stowe, H. M.; Yu, J.; Hwang, G. S. "First-Principles Prediction of Iron(II)-Assisted Carbon Dioxide Conversion to Formate in Aqueous Amines." *In-preparation.*

2. **Yoon, B.**; Yu, J.; Calabro, D. C.; Saunders, L.; Raman, S.; Hwang, G. S. "Steric Hindrance Effects on the Thermal Degradation of Aqueous Alkanolamines for Carbon Dioxide Capture: A First-Principles Assessment." *In-preparation.*

1. **Yoon, B.**; Voth, G. A. "On the Influence of Water Contents in Amino Acid Ionic Liquids for CO2 Capture." *In-preparation.*

Conference Proceedings and Presentations

23. *[Sep 2024]* **Yoon, B.** "Materials Design and Discovery of Biocompatible Ionic Liquids for CO2 Direct Air Capture and Conversion." Seminar Talk, Korea University, Seoul, South Korea. [**Invited**]

22. *[Sep 2024]* **Yoon, B.** "Computational Design and Discovery of Biocompatible Materials for CO2 Direct Air Capture and Conversion." Seminar Talk, Ewha Womans University, Seoul, South Korea. [**Invited**]

21. *[Aug 2024]* **Yoon, B.** "Biocompatible Ionic Liquids: In Silico Approach to Energy and Sustainability Challenges in CO2 Direct Air Capture and Conversion." Gordon Research Conference (GRC), Ionic Liquids, 2024, Newry, ME. [**Poster Award**]

20. *[Jul 2024]* **Yoon, B.** "In Silico Materials Design and Discovery for Energy and Sustainability: Biocompatible Solutions for CO2 Direct Air Capture and Conversion." Seminar Talk, Soongsil University, Seoul, South Korea. **[Invited]**

19. *[Jul 2024]* **Yoon, B.** "In Silico Materials Design and Discovery for Energy and Sustainability: Biocompatible Solutions for CO2 Direct Air Capture and Conversion." Seminar Talk, Inha University, Incheon, South Korea. **[Invited]**

18. *[May 2024]* **Yoon, B.** "Next-Generation Materials Design for CO2 Direct Air Capture and Conversion." Northwestern University Theoretical Chemistry Seminar Series, Evanston, IL. **[Invited]** [link]

17. *[Mar 2024]* **Yoon, B.**; Voth, G. A. "Materials Design of Amino Acid Ionic Liquids for CO2 Capture and Conversion: A Multiscale Theory/Modeling." ACS Spring 2024, New Orleans, LA.

16. *[Nov 2023]* **Yoon, B.** "Computation- and Theory-Guided Materials Discovery and Design for CO2 Capture, Utilization, and Storage." 2023 AIChE Annual Meeting, Orlando, FL. [link]

15. *[Nov 2023]* **Yoon, B.**; Voth, G. A. "A Multiscale Approach Toward Direct Air Capture of CO2 by Biocompatible Ionic Liquids." 2023 AIChE Annual Meeting, Orlando, FL. [link]

14. *[Nov 2023]* **Yoon, B.**; Calabro, D. C.; Saunders, L.; Raman, S.; Hwang, G. S. "Engineering Aqueous Amine Solvents Based on Steric Effects for CO2 Capture from First-Principles Simulations." 2023 AIChE Annual Meeting, Orlando, FL. [link]

13. *[Aug 2023]* **Yoon, B.**; Voth, G. A. "On the Structural, Dynamic, and Reactive Properties of CO2 Capture by Biocompatible Ionic Liquids: Theory and Computer Simulations." Gordon Research Conference (GRC), Chemistry and Physics of Liquids, 2023, Holderness, NH.

12. *[Jul 2023]* **Yoon, B.** "Mechanistic Insights into CO2 Capture by Amino Acid Ionic Liquids through Multiscale Simulations." The Chicago Center for Theoretical Chemistry (CCTCh) at the University of Chicago 2023, Chicago, IL. **[Invited]** [link]

11. *[Jul 2023]* **Yoon, B.** "A Multiscale Simulation Approach on the Structural, Dynamic, and Reactive Properties of Biocompatible Ionic Liquids on CO2 Capture." Seminar Talk, Korea Institute of Science and Technology (KIST), Seoul, South Korea. **[Invited]**

10. *[Jul 2023]* **Yoon, B.**; Voth, G. A. "CO2 Capture by Biocompatible Ionic Liquids: Computation and Theory." Gordon Research Seminar (GRS), Chemistry and Physics of Liquids, 2023, Holderness, NH.

9. *[Jun 2022]* **Yoon, B.** "First-Principles Studies on Degradation of Aqueous Amine Solvents for CO2 Capture." Seminar Talk, Korea Institute of Science and Technology (KIST), Seoul, South Korea. **[Invited]**

8. *[Mar 2022]* **Yoon, B.**; Hwang, G. S. "First-Principles Assessment of Thermal Degradation Mechanisms of Aqueous Piperazine (PZ) for CO2 Capture." ACS Spring 2022, San Diego, CA.
DOI: 10.1021/scimeetings.2c00107

7. *[Jan 2022]* **Yoon, B.**; Hwang, G. S. "First-Principles Comparative Study of Thermal Degradation of Aqueous Amine Solvents for CO2 Capture." 2022 University of Texas Conference on Carbon Capture and Storage (UTCCS) 6th Conference, Austin, TX.

6. *[Nov 2021]* **Yoon, B.**; Hwang, G. S. "First-Principles Insights into Thermal Degradation Mechanisms of Aqueous 2-Amino-2-methyl-1-propanol (AMP) for CO2 Capture." 2021 AIChE Annual Meeting, Boston, MA. [link]

5. *[Aug 2021]* **Yoon, B.**; Hwang, G. S. "On the Critical Role of Arrangement and Dynamics of Water Molecules in CO2 Capture by Aqueous Amines." ACS Fall 2021, Atlanta, GA. DOI: 10.1021/scimeetings.1c00931

4. *[Apr 2021]* **Yoon, B.**; Hwang, G. S. "On the Origin of Peculiar Facile Carbamate Formation at High Stripping Temperatures from CO2 Capture in Aqueous 2-Amino-2-methyl-1-propanol." ACS Spring 2021, Virtual.
DOI: 10.1021/scimeetings.1c00713

3. *[Nov 2020]* **Yoon, B.**; Hwang, G. S. "First-Principles Modeling of Thermal Degradation of CO2-Loaded Aqueous Amine Solvents." 2020 Virtual AIChE Annual Meeting. [link]

2. *[Nov 2020]* **Yoon, B.**; Hwang, G. S. "Revealing the Mechanism of Intriguing Predominant Urea Formation from Thermal Degradation of CO2-Loaded Aqueous Ethylenediamine." 2020 Virtual AIChE Annual Meeting. [link]

1. *[Jan 2022]* **Yoon, B.**; Hwang, G. S. "Molecular Modeling of 3,3'-Iminobis (N,N-Dimethylpropylamine) (IB-DMPA)." 2020 University of Texas Conference on Carbon Capture and Storage (UTCCS) 5th Conference, Austin, TX.

Research Experiences

The University of Chicago *2022-2024*
Postdoctoral Fellow in Theoretical Chemistry with Dr. Gregory A. Voth
Title: *"Multiscale Simulations of Ionic Liquids for Sustainability Challenges"*

The University of Texas at Austin *2017-2022*
Graduate Research Assistant in Chemical Engineering with Dr. Gyeong S. Hwang
Dissertation: *"First-Principles Studies on Degradation of Aqueous Amines for Carbon Dioxide Capture"*

Lehigh University *2014-2016*
Undergraduate Research Assistant in Chemical Engineering with Dr. Mark A. Snyder
Thesis: *"Nanocasting of Bicontinuous 3-D Ordered Mesoporous Carbon Films by Template Replica Co-Assembly"*

Teaching Experiences

The University of Chicago, Department of Chemistry *Spring 2024*
Lecturer, *Quantum Chemistry I*

The University of Texas at Austin, Department of Chemical Engineering *Fall 2019, Spring 2018, Fall 2017*
Graduate Teaching Assistant (for three semesters), *Transport Phenomena*

Lehigh University, Department of Chemical Engineering

Undergraduate Teaching Assistant, *Chemical Reaction Kinetics & Reactor Design*	*Spring 2016*
Undergraduate Teaching Assistant, *Numerical Methods of Analysis*	*Summer 2015*
Undergraduate Teaching Assistant, *Fluid Mechanics*	*Spring 2015*
Undergraduate Teaching Assistant, *Heat Transfer*	*Fall 2014*

Honors, Awards, and Fellowships

Poster Award, Gordon Research Conference (GRC) Ionic Liquids 2024	*2024*
Kharasch Chemistry Postdoctoral Fellowship, The University of Chicago	*2022-2024*
Harry and Rubye Gaston Graduate Scholarship, The University of Texas at Austin	*2021-2022*
Professional Development Award, The University of Texas at Austin	*2020-2022*
James R. & Merle Fair Endowed Fellowship, The University of Texas at Austin	*2020*
2nd Place, 1st/3rd Year Graduate Student Seminar Series in Chemical Engineering	*2020*
Dean's List (All semesters), Lehigh University	*2010-2016*
Teaching Assistant of the Year Award, Lehigh University	*2015*
Tau Beta Pi (National Honors Engineering Society), Lehigh University	*2014*
The National Society of Collegiate Scholars	*2011*

Reviewed/Refereed for Peer-Reviewed Journals

J. Phys. Chem. Lett.; J. Phys. Chem. B.; Ind. Eng. Chem. Res.; Phys. Chem. Chem. Phys.; ACS Sustainable. Chem. Eng.; J. Chem. Phys.; Chem. Eng. J.

References

Gregory A. Voth, Ph.D. | *Postdoctoral Advisor*
Haig P. Papazian Distinguished Service Professor of Chemistry, The University of Chicago
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Gyeong S. Hwang, Ph.D. | *Ph.D. Advisor*
Mathew Van Rickel Professor of Chemical Engineering, The University of Texas at Austin
Phone: 512-471-4847 | Email: gshwang@che.utexas.edu

Pengyu Ren, Ph.D. | *Ph.D. Thesis Committee*
E.C.H. Bantel Professor in Biomedical Engineering, The University of Texas at Austin
Phone: 512-232-1832 | Email: pren@mail.utexas.edu

Steven McIntosh, Ph.D. | *Undergraduate Advisor*
Professor and Department Chair of Chemical and Biomolecular Engineering, Lehigh University
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