

Thomas P. Senftle

Department of Chemical Biomolecular Engineering
 Rice University
 tsenftle@rice.edu

Education:

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| The Pennsylvania State University , University Park, PA | 2015 |
| <i>Doctor of Philosophy</i> – Chemical Engineering, Department of Chemical Engineering | |
| University of Notre Dame , South Bend, IN | 2010 |
| <i>Bachelor of Science</i> – Chemical Engineering (Major), Department of Chemical and Biomolecular Engineering
Philosophy (Supplemental Major), Department of Philosophy | |

Academic Positions:

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- | | |
|---|-------------|
| Rice University , Houston, TX | 2017 – |
| <i>Assistant Professor</i>
Department of Chemical and Biomolecular Engineering
George R. Brown School of Engineering | |
| Princeton University , Princeton, NJ | 2015 – 2017 |
| <i>Postdoctoral Research Associate</i>
Advisor: Prof. Emily A. Carter, Department of Mechanical and Aerospace Engineering | |
| The Pennsylvania State University , University Park, PA | 2010 – 2015 |
| <i>Graduate Research Assistant</i>
Advisors: Prof. Michael J. Janik, Department of Chemical Engineering
Prof. Adri van Duin, Department of Mechanical and Nuclear Engineering | |
| The University of Notre Dame , South Bend, IN | 2008 – 2010 |
| <i>Undergraduate Research Assistant</i>
Advisor: Prof. William F. Schneider, Department of Chemical and Biomolecular Engineering | |

Publications: [Google Scholar](#) – Citations: 3732, h-index: 25

Students advised by T. P. Senftle are underlined.

A PDF of each paper can be found at <https://senftle.blogs.rice.edu/publications>

53. Ye, S.; **Senftle, T.P.**; Li, M.*, "Operator-induced structural variable selection with applications to materials genomes." *Submitted*. arXiv: 2110.10195
52. Wang, P.; **Senftle, T. P.***, "Addressing challenges in modeling complex structures in heterogeneous catalysis." (Book Chapter) *Computational Catalysis, 2nd Ed.*, 2023, Royal Society of Chemistry. (In Press)
51. Zhu, D.; Zhu, Y.; Chen, Y.; Yan, Q.; Wu, H.; Liu, C.-Y.; Wang, X.; Alemany, L. B.; Gao, G.; **Senftle, T. P.**; Peng, Y.; Wu, X.*; Verduzco, R.*, "Three-dimensional covalent organic frameworks with pto and mhq-z topologies based on Tri- and tetratopic linkers." *Nature Communications* 2023 *Accepted*. DOI: 10.1038/s41467-023-38538-x

50. Rehn, S. M.; Gerrard-Anderson, T. M.; Chen, Y.; Wang, P.; Robertson, T.; **Senftle, T. P.**; Jones, M. R.*, "Surface ligands dictate the mechanical properties of inorganic nanomaterials." *ACS Nano* 2023, 17 (7), 6698.
49. Bhati, M.; Ivanov, S. A.; **Senftle, T. P.**; Tretiak, S.*; Ghosh, D.*, "How structural and vibrational features affect optoelectronic properties of non-stoichiometric quantum dots: computational insights." *Nanoscale* 2023, 15, 7176.
48. Lim, J.; Chen, Y.; Cullen, D.; Lee, S. W.; **Senftle, T. P.***; Hatzell, M.*, "PdCu electrocatalysts for selective nitrate and nitrite reduction to nitrogen." *ACS Catalysis* 2023, 13 (1), 87.
47. Duan, L.; Wang, B.; Heck, K. N.; Clark, C. A.; Wei, J.; Wang, M.; Metz, J.; Wu, G.; Tsai, A.-L.; Guo, S.; Arredondo, J.; Mohite, A. D.; **Senftle, T. P.**; Westerhoff, P.; Alvarez, P.; Wen, X.; Song, Y.*; Wong, M. S.*, "Titanium oxide improves boron nitride photocatalytic degradation of perfluorooctanoic acid." *Chemical Engineering Journal* 2022, 448, 137735.
46. Carrón-Calle, G.; **Senftle, T. P.**, Garcia-Segura, S.*, "Strategic tailored design of electrocatalysts for environmental remediation based on density functional theory (DFT) and microkinetic modelling." *Current Opinion in Electrochemistry* 2022, 35, 101062.
→ **Invited:** Special Issue: Emerging Opinions (2022)
45. Chen, Y.; Bhati, M.; Walls, B. W.; Wang, B.; Wong, M. S.; **Senftle, T. P.***, "Mechanistic insight into the photo-oxidation of perfluorocarboxylic acid over hexagonal boron nitride." *Environmental Science and Technology* 2022, 56 (12), 8942.
44. Liu, C.-Y.; **Senftle, T. P.***, "Finding physical insights in catalysis with machine learning." *Current Opinion in Chemical Engineering* 2022, 37, 100832.
→ **Invited:** Special Issue: Data Centric Catalysis and Reaction Engineering
43. Lyu, Y.; Wang, P.; Liu, D.; Zhang, F.; **Senftle, T. P.***; Zhang, G.; Zhang, Z.*; Wang, J.; Liu, W.*, "Tracing the active phase and dynamics for carbon nanofiber growth on nickel catalyst using environmental transmission electron microscopy." *Small Methods* 2022, 6, 2200235.
42. Liu, C.-Y.; Ye, S.; Li, M.*; **Senftle, T. P.***, "A rapid feature selection method for catalyst design: Iterative Bayesian additive regression trees (iBART)" *Journal of Chemical Physics* 2022, 156, 164105.
→ **Invited:** JCP Special Topic on Chemical Design by Artificial Intelligence
41. Bhati, M.; Ivanov, S. A.; **Senftle, T. P.**; Tretiak, S.*; Ghosh, D.*, "Nature of electronic excitations in non-stoichiometric quantum dots." *Journal of Materials Chemistry A* 2022, 10 (10), 5003.
40. Zhu, J.; Wang, P.; Zhang, X.; Zhang, G.*; Li, R.; Li, W.; **Senftle, T. P.**; Liu, W.; Wang, J.; Wang, Y.; Zhang, A.; Fu, Q.; Song, C.; Guo, X.*, "Dynamic structural evolution of iron catalysts involving competitive oxidation and carburization during CO₂ hydrogenation." *Science Advances* 2022, 8 (5), abm3629.
39. Fan, L.; Liu, C.-Y.; Zhu, P.; Xia, C.; Zhang, X.; Wu, Z.-Y.; Lu, Y.*; **Senftle, T. P.***; Wang, H.*, "Proton sponge promotion of electrochemical CO₂ reduction to multi-carbon products." *Joule* 2022, 6 (1), 205.
38. Zhu, Y.; Zhu, D.; Chen, Y.; Yan, Q.; Liu, C.-Y.; Ling, K.; Liu, Y.; Lee, D.; Wu, X.*; **Senftle, T. P.***; Verduzco, R.*, "Porphyrin-based donor-acceptor COFs as efficient and reusable photocatalysts for PET-RAFT polymerization under broad spectrum excitation." *Chemical Science* 2021, 12, 16092.
37. Long, M.; Elias, W. C.; Heck, K. N.; Luo, Y.-H.; Lai, Y. S.; Jin, Y.; Gu, H.; Donoso, J.; **Senftle, T. P.**; Zhou, C.*; Wong, M. S.; Rittmann, B. E., "Hydrodefluorination of perfluorooctanoic acid in the H₂-based membrane catalyst-film reactor with platinum group metal nanoparticles: Pathways and optimal conditions." *Environmental Science and Technology* 2021, 55 (24), 16699.
36. Long, M.; Donoso, J.; Bhati, M.; Elias, W. C.; Heck, K. N.; Luo, Y.-H.; Lai, Y. S.; Gu, H.; **Senftle, T. P.**; Zhou, C.*; Wong, M. S.; Rittmann, B. E., "Adsorption and reductive defluorination of perfluorooctanoic acid (PFOA) over palladium nanoparticles." *Environmental Science and Technology* 2021, 55 (21), 14836.
35. Wang, P.; **Senftle, T. P.***, "Modeling phase formation on catalyst surfaces: Coke formation and suppression in hydrocarbon environments." *AIChE Journal* 2021, 67 (12), e17454.
→ **Invited:** AIChE Journal special issue "AIChE Futures"

34. **Bhati, M.**; Nguyen, Q. A.; Biswal, S. L.; **Senftle, T. P.***, “Combining ReaxFF simulation and experiment to evaluate the structure-property characteristics of polymeric binders in Si-based Li-ion batteries.” *ACS Applied Materials and Interfaces* 2021, 13 (35), 41956.
33. Lim, J.; **Liu, C.-Y.**; Park, J.; Liu, Y.-H.; **Senftle, T. P.***; Lee, S. W.*; Hatzell, M. C.*, “Structure sensitivity of Pd facets for enhanced electrochemical nitrate reduction to ammonia.” *ACS Catalysis* 2021, 11 (12), 7568.
32. Zhu, P.; Xia, C., **Liu, C.-Y.**; Jiang, K.; Gao, G.; Zhang, X.; Xia, Y.; Lei, Y.; Alshareef, H. N.; **Senftle, T. P.***; Wang, H.*, “Direct and continuous generation of pure acetic acid solutions via electrocatalytic carbon monoxide reduction.” *Proceedings of the National Academy of Sciences* 2021, 118 (2), e2010868118.
31. **Wang, P.**; **Senftle, T. P.***, “Theoretical insights into non-oxidative propane dehydrogenation over Fe₃C.” *Physical Chemistry Chemical Physics* 2021, 23 (2), 1401.
30. **Bhati, M.**; **Chen, Y.**; **Senftle, T. P.***, “Density functional theory modeling of photo-electrochemical reactions on semiconductors: H₂ evolution on 3C-SiC.” *Journal of Physical Chemistry C* 2020, 124 (49), 26625.
→ **Invited:** The Journal of Physical Chemistry virtual special issue “Emily A. Carter Festschrift”
29. **Liu, C.-Y.**; Zhang, S.; **Martinez, D.**; Li, M.*; **Senftle, T. P.***, “Using statistical learning to predict interactions between single metal atoms and modified MgO(100) supports.” *npj Computational Materials* 2020, 6 (1), 1.
28. Duan, L.; Wang, B.; Heck, K.; Guo, S.; Clark, C. A.; Arredondo, J.; Wang, M.; **Senftle, T. P.**; Westerhoff, P.; Wen, X.; Song, Y.; Wong, M. S.*, “Efficient photocatalytic PFOA degradation over boron nitride.” *Environmental Science & Technology Letters* 2020, 7 (8), 613.
27. Wang, J.; **Liu, C.-Y.**; **Senftle, T. P.**; Zhu, J.; Zhang, G.*; Guo, X.*; Song, C.*, “Variation in In₂O₃ crystal phase alters catalytic performance toward the reverse water gas shift reaction.” *ACS Catalysis* 2020, 10 (5), 3264.
26. Clark, C. A., **Reddy, C. P.**; Xu, H.; Heck, K. N.; Luo, G.; **Senftle, T. P.***; Wong, M. S.*, “Mechanistic insights into pH-controlled nitrite reduction to ammonia and hydrazine over rhodium.” *ACS Catalysis* 2020, 10 (1), 494.
25. **Bhati, M.**; **Senftle, T. P.***, “Identifying adhesion properties at Si/polymer interfaces with ReaxFF.” *Journal of Physical Chemistry C* 2019, 123 (44) 27036.
24. O’Connor, N.; Jonayat, A. S. M.; Janik, M.J.*; **Senftle, T. P.***, “Interaction trends between single metal atoms and oxide supports identified with density functional theory and statistical learning.” *Nature Catalysis* 2018, 1 (7), 531.
23. Gautam, G. S.; **Senftle, T. P.**; Alidoust, N.; Carter, E. A.*, “Novel solar cell materials: insights from first-principles” *Journal of Physical Chemistry C* 2018, 122 (48), 27107.
22. Gautam, G. S.; **Senftle, T. P.**; Carter, E. A.*, “Understanding the effects of Cd and Ag doping in Cu₂ZnSnS₄ solar cells.” *Chemistry of Materials* 2018, 30 (14), 4543.
21. Lessio, M.; **Senftle, T. P.**; Carter, E. A.*, “Hydride shuttle formation and reaction with CO₂ on GaP(110).” *ChemSusChem* 2018, 11 (9), 1588.
20. **Senftle, T. P.**; Lessio, M.; Carter, E. A.*, “The role of surface-bound dihydropyridine analogues in pyridine-catalyzed CO₂ reduction over semiconductor photoelectrodes.” *ACS Central Science* 2017, 3 (9), 968.

Before appointment at Rice University

19. **Senftle, T. P.**; Carter, E. A. “Theoretical determination of band edge alignments at the water–CuInS₂(112) semiconductor interface.” *Langmuir* 2017, 33 (37), 9479.
18. **Senftle, T. P.**; Carter, E. A. “The Holy Grail: Chemistry enabling an economically viable CO₂ capture, utilization, and storage strategy.” *Accounts of Chemical Research* 2017, 50 (3), 472.

17. Fantauzzi, D.; Krick Calderón, S.; Mueller, J. E.; Grabau, M.; Papp, C.; Steinrück, H.-P.; **Senftle, T. P.**; van Duin, A. C. T.; Jacob, T. "Growth of stable surface oxides on Pt(111) at near-ambient pressures." *Angewandte Chemie International Edition* 2017, 56 (10), 2594.
16. **Senftle, T. P.**; van Duin, A. C. T.; Janik, M. J. "Methane activation at the Pd/CeO₂ interface." *ACS Catalysis* 2016, 7 (1), 327.
15. **Senftle, T. P.**; Lessio, M.; Carter, E.A., "Interaction of pyridine and water with the reconstructed surfaces of GaP(111) and CdTe(111) photoelectrodes: Implications for CO₂ reduction." *Chemistry of Materials* 2016, 28 (16), 5799.
14. Lessio, M.; **Senftle, T. P.**; Carter, E.A., "Is the surface playing a role during pyridine-catalyzed CO₂ reduction on p-GaP photo-electrodes?" *ACS Energy Letters* 2016, 1 (2), 464.
13. **Senftle, T. P.**; Hong, S.; Islam, M. M.; Kylasa, S. B.; Zheng, Y.; Shin, Y. K.; Junkermeier, C.; Engel-Herbert, R.; Janik, M. J.; Aktulga, H. M.; Verstraelen, T.; Grama, A.; van Duin, A. C. T., "The ReaxFF reactive force-field: development, applications and future directions." *npj Computational Materials* 2016, 2, 15011.
12. **Senftle, T. P.**; van Duin, A. C. T.; Janik, M. J., "Role of site stability in describing methane activation on Pd_xCe_{1-x}O₈." *ACS Catalysis* 2015, 5 (10), 6187.
11. Strayer, M. E.; **Senftle, T. P.**; Winterstein, J. P.; Vargas-Barbosa, N. M.; Sharma, R.; Janik, M. J.; Mallouk, T. E., "Charge transfer stabilization of late transition metal oxide nanoparticles on a layered niobate support." *Journal of the American Chemical Society* 2015, 137 (51), 16216.
10. Tavazza, F.; **Senftle, T. P.**; Zou, C.; Becker, C. A.; van Duin, A. C. T., "Molecular dynamics investigation of the effects of tip-substrate interactions during nanoindentation." *Journal of Physical Chemistry C* 2015, 119 (24), 13580.
9. **Senftle, T. P.**; Janik, M. J.; van Duin, A. C. T., "A ReaxFF Investigation of hydride formation in Pd nanoclusters via Monte Carlo and molecular dynamics simulations." *Journal of Physical Chemistry C* 2014, 118 (9), 4967.
8. Addou, R.; **Senftle, T. P.**; O'Connor, N.; Janik, M. J.; van Duin, A. C. T.; Batzill, M., "Influence of hydroxyls on Pd atom mobility and clustering on rutile TiO₂(011)-(2×1)." *ACS Nano* 2014, 8 (6), 6321.
7. Spanjers, C. S.; **Senftle, T. P.**; van Duin, A. C. T.; Janik, M. J.; Frenkel, A. I.; Rioux, R. M., "Illuminating surface atoms in nanoclusters by differential X-ray absorption spectroscopy." *Physical Chemistry Chemical Physics* 2014, 16 (48), 26528.
6. **Senftle, T. P.**; van Duin, A. C. T.; Janik, M. J., "Application of computational methods to supported metal-oxide catalysis." (Book Chapter) *Computational Catalysis* 2014, Royal Society of Chemistry, p. 157.
5. **Senftle, T. P.**; Meyer, R. J.; Janik, M. J.; van Duin, A. C. T., "Development of a ReaxFF potential for Pd/O and application to palladium oxide formation." *Journal of Chemical Physics* 2013, 139 (4), 044109.
4. **Senftle, T. P.**; van Duin, A. C. T.; Janik, M. J., "Determining *in situ* phases of a nanoparticle catalyst via grand canonical Monte Carlo simulations with the ReaxFF potential." *Catalysis Communications* 2013, 52 (0), 72.
3. Wu, C.; **Senftle, T. P.**; Schneider, W. F., "First-principles-guided design of ionic liquids for CO₂ capture." *Physical Chemistry Chemical Physics* 2012, 14 (38), 13163.
2. Hudgens, J. W.; Pettibone, J. M.; **Senftle, T. P.**; Bratton, R. N., "Reaction mechanism governing formation of 1,3-Bis(diphenylphosphino)propane-protected gold nanoclusters." *Inorganic Chemistry* 2011, 50 (20), 10178.
1. Gurkan, B.; Goodrich, B. F.; Mindrup, E. M.; Ficke, L. E.; Massel, M.; Seo, S.; **Senftle, T. P.**; Wu, H.; Glaser, M. F.; Shah, J. K.; Maginn, E. J.; Brennecke, J. F.; Schneider, W. F., "Molecular design of high capacity, low viscosity, chemically tunable ionic liquids for CO₂ capture." *Journal of Physical Chemistry Letters* 2010, 1 (24), 3494.

Seminars, Lectures, and Conference Presentations:

Invited

‡ - Indicates a scheduled talk.

1. ‡ “Mechanistic insight into photo-catalytic PFAS degradation mechanisms.”
American Chemical Society National Meeting. San Francisco CA, August 2023.
2. ‡ “Constructing physical descriptors in catalysis with iterative symbolic regression.”
American Chemical Society National Meeting. San Francisco CA, August 2023.
3. ‡ “The role of computational chemistry in designing clean energy technologies.”
Tapia Center-Molecule Sciences Software Institute (Tapia-MolSSI): Workshop in Computational Chemistry. Houston TX, June 2023.
4. “Designing oxide-based catalysts for the electrochemical oxidation of hydrocarbons with insights from statistical learning.”
American Chemical Society National Meeting. Indianapolis IN, March 2023.
5. “Implications of *in situ* phase transformations in CO₂ hydrogenation catalysis.”
American Chemical Society National Meeting. Indianapolis IN, March 2023.
6. “Understanding Metal-Support Interactions in Catalysis with Statistical Learning.”
Penn State University, Department of Chemical Engineering, Seminar. October 2022.
7. “Understanding Metal-Support Interactions in Catalysis with Statistical Learning.”
Rice University, Department of Computational Applied Mathematics and Operations Research, Seminar. Houston, TX, December 2022.
8. “Understanding metal/support interactions in catalysis with statistical learning.”
Dalian University of Technology, Catalysis Group, Seminar. Virtual, May 2022.
9. “The role of computational chemistry in designing clean energy technologies.”
Tapia Center-Molecule Sciences Software Institute (Tapia-MolSSI): Workshop in Computational Chemistry. Houston TX, June 2022.
10. “Mechanistic Insight into the Electrocatalytic Reduction of Nitrate to Ammonia”
241st Electrochemical Society Meeting in Vancouver, BC, Canada. Virtual, May 2022.
11. “Understanding Interfaces in Electrochemical Systems with Atomistic Simulation.”
Workshop Series: Where is Energy Storage Headed? Interfacial Phenomena in Electrochemical Systems. Boston University, Institute for Sustainable Energy. Virtual, January 2022.
12. “Modeling phase formation on catalyst surfaces: Coke formation and suppression in hydrocarbon environments.”
American Institute of Chemical Engineers National Meeting. Boston MA, November 2021. (Invited as part of the symposium titled *AIChE Journal Futures: New Directions in Chemical Engineering Research*)
13. “Constructing physical descriptors in catalysis with statistical learning.”
American Chemical Society National Meeting. Atlanta GA, August 2021.
14. “Multi-scale modeling tools for designing water treatment technologies.”
Nanosystems Engineering Research Center for Nanotechnology Enables Water Treatment (NEWTE): Computational Chemistry Workshop. Houston TX, August 2021.
15. “Computational chemistry: Tools for designing clean energy technologies.”
Tapia Center-Molecule Sciences Software Institute (Tapia-MolSSI): Workshop in Computational Chemistry. Houston TX, July 2021.
16. “Understanding metal-support interactions in catalysis with statistical learning.”

Rice University, Department of Chemical and Biomolecular Engineering, Seminar. Houston TX, October 2020.

17. "Identifying physical descriptors with statistical learning for predicting metal-support interactions in catalysis." *UOP-Honeywell Invitational Lecture Series.* Des Plains IL, May 2019.
18. "Identifying physical descriptors for predicting metal-support interactions in catalysis with DFT and statistical learning." *Southwest Catalysis Society Spring Symposium.* Houston TX, April 2019.
19. "Identifying physical descriptors for predicting metal-support interactions in catalysis." *American Chemical Society National Meeting.* Orlando FL, April 2019.

Contributed

Students advised by T. P. Senftle are underlined.

1. Chen, Y.; **Senftle, T. P.**, "Theoretical insights into the photocatalytic PFOA degradation mechanism over boron nitride." *American Institute of Chemical Engineers National Meeting.* Phoenix AZ, November 2022.
2. Chen, Yu; Bhati, M.; Walls, B.; **Senftle, T. P.**, "Mechanistic insight into the photo-catalytic degradation of PFOA over boron nitride." (Poster) *Gordon Research Conference on Catalysis.* New London VT, June 2022.
3. Chen, Yu; Bhati, M.; **Senftle, T.P.**, "Theoretical insight into photo-catalytic PFAS degradation mechanisms over boron nitride." *American Institute of Chemical Engineers National Meeting.* Boston MA, November 2021.
4. Reddy, P.; Clark, C. A.; Heck, K. N.; Wong, M. S.; **Senftle, T. P.**, "Mechanistic insights into pH-controlled nitrite reduction to ammonia over rhodium." *American Institute of Chemical Engineers National Meeting.* Virtual, November 2020.
5. Liu, C.-Y.; **Senftle, T. P.**, "Using statistical learning to identify physical descriptors that predict metal-support interactions in catalysis." *North American Catalysis Society Meeting.* Chicago, IL, June 2019.
6. **Senftle, T. P.**, "Unraveling metal-support interactions with DFT and statistical learning." *American Institute of Chemical Engineers National Meeting.* Pittsburgh PA, October 2018.
7. **Senftle, T. P.**, "Physical descriptors that control metal-support interactions identified with DFT and machine learning." (Poster) *Gordon Research Conference on Catalysis.* New London VT, June 2018.
8. **Senftle, T. P.**; Carter, E. A., "The role of surface-bound dihydropyridine analogs in pyridine-catalyzed CO₂ reduction over semiconductor photoelectrodes." *American Institute of Chemical Engineers National Meeting.* Minneapolis MN, October 2017.

Before Appointment at Rice University

9. **Senftle, T. P.**; Carter, E. A., "The holy grail: chemistry enabling an economically viable CO₂ capture, utilization, and storage strategy." (Poster) *American Chemical Society National Meeting.* San Francisco CA, April 2017.
10. **Senftle, T. P.**; Carter, E. A., "Pyridine Co-catalysis impacting CO₂ reduction over semiconductor photoelectrodes." *American Chemical Society National Meeting.* San Francisco CA, April 2017.
11. **Senftle, T. P.**; Carter, E. A., "How do surface reconstructions affect CO₂ reduction over GaP, CdTe, and CuInS₂ photo-electrodes?" *American Chemical Society National Meeting.* San Diego CA, March 2016.
12. **Senftle, T. P.**; van Duin, A. C. T.; Janik, M. J., "Methane activation at the Pd/CeO₂ interface." *North American Meeting of the Catalysis Society.* Pittsburg PA, June, 2015.
13. **Senftle, T. P.**; van Duin, A. C. T.; Janik, M. J., "Investigation of interfacial oxide activity and stability on Pd/CeO₂ catalysts." *American Chemical Society National Meeting.* Denver CO, March, 2015.

14. **Senftle, T. P.**; van Duin, A. C. T.; Janik, M. J., "Multi-Scale investigation of Pd/Ceria catalysts *via* density functional theory and classical ReaxFF simulations." *American Institute of Chemical Engineers National Meeting*. Atlanta GA, November, 2014.
15. **Senftle, T. P.**; van Duin, A. C. T.; Janik, M. J., "Screening for active sites on supported metal-oxide catalysts *via* hybrid Monte Carlo/molecular dynamics simulations with the ReaxFF potential." *American Institute of Chemical Engineers National Meeting*. Atlanta GA, November, 2014.
→ Selected as Best Presentation in the session "Rational Catalyst Design II"
16. **Senftle, T. P.**; van Duin, A. C. T.; Janik, M. J., "Multi-scale investigation of oxide formation on Pd/Ceria catalysts *via* DFT and ReaxFF simulations." (Poster) *Gordon Research Conference on Catalysis*. New London VT, June 2014.
→ Awarded Gary McVicker Poster Award (2nd Place)
17. **Senftle, T. P.**; van Duin, A. C. T.; Janik, M. J., "Development of hybrid-MD/MC methods to investigate oxide formation on Pd-based catalysts." *Spring Meeting of the Pittsburgh Cleveland Catalysis Society*. Pittsburgh PA, May 2013.
18. **Senftle, T. P.**; van Duin, A. C. T.; Janik, M. J., "Multi-scale DFT/ReaxFF modeling of Ceria supported Pd catalysts" *American Institute of Chemical Engineers National Meeting*. Pittsburgh PA, October, 2012.
19. **Senftle, T. P.**; van Duin, A. C. T.; Janik, M. J., "Reactive force-field development for modeling of Pd/Ceria catalysts." *American Chemical Society National Meeting*. Philadelphia PA, August 2012.
20. **Senftle, T. P.**; van Duin, A. C. T.; Janik, M. J., "Computational characterization of Pd/Ceria catalysts using DFT+U and ReaxFF." *American Institute of Chemical Engineers National Meeting*. Minneapolis MN, October 2011.

Presentations by Advised Students

Students advised by T. P. Senftle are underlined. Presenter is italicized.

1. Chen, Y.; **Senftle, T. P.**, "Theoretical insights into the photocatalytic PFOA degradation mechanism over boron nitride." *American Institute of Chemical Engineers National Meeting*. Phoenix AZ, November 2022.
2. Chen, Y.; **Senftle, T. P.**, "Theoretical methods for assessing the feasibility of PFOA oxidation on photocatalyst surfaces." (Poster) *American Institute of Chemical Engineers National Meeting*. Phoenix AZ, November 2022.
3. Walls, B.; **Senftle, T. P.**, "Learning metal/support interactions in single-atom catalysts with symbolic regression." *American Institute of Chemical Engineers National Meeting*. Phoenix AZ, November 2022.
→ Awarded *Best Student Presentation*
4. Wang, P.; **Senftle, T. P.**, "Selectivity and activity of Fe₃C as a propane dehydrogenation catalyst." *American Institute of Chemical Engineers National Meeting*. Phoenix AZ, November 2022.
5. Walls, B.; **Senftle, T. P.**, "Understanding physical descriptors in catalysis with machine learning." AICHe Southwest Regional Conference. Austin TX, March 2022.
→ Awarded first place in *Best Presentation* competition
6. Chen, Y.; **Senftle, T. P.**, "Hydrophobicity of hBN enhances its photocatalytic PFOA degradation performance." *American Chemical Society National Meeting*. Virtual, March 2022.
7. Bhati, M.; **Senftle, T. P.**, "Bhati, M.; Senftle, T. P., "Designing high-performing binders for Si anodes in Li-ion batteries." (Poster) *American Chemical Society National Meeting*. Virtual, March 2022.
→ Winner of the ENFL Student Poster Award Competition 2022
8. Bhati, M.; **Senftle, T. P.**, "Bhati, M.; Senftle, T. P., "Investigating binder materials for Si anode in Li-ion battery using reactive force fields." *American Chemical Society National Meeting*. Virtual, March 2022.
9. Liu, C.-Y.; Ye, S.; Li, M.; **Senftle, T. P.**, "Building Catalytic Descriptors with Iterative Bayesian Additive Regression Trees (iBART)." *American Institute of Chemical Engineers National Meeting*. Boston MA, November 2021.
10. Liu, C.-Y.; Ye, S.; Li, M.; **Senftle, T. P.**, "Improving Feature Selection Methods for Heterogeneous

- Catalysis.” (Poster) *American Institute of Chemical Engineers National Meeting*. Boston MA, November 2021.
11. Wang, P.; **Senftle, T. P.**, “Designing coke-resistant dehydrogenation catalysts with DFT and grand canonical Monte Carlo simulations.” *American Institute of Chemical Engineers National Meeting*. Boston MA, November 2021.
 12. Wang, P.; **Senftle, T. P.**, “Grand canonical Monte Carlo simulation methods for understanding coke-resistance under dehydrogenation conditions.” (Poster) *American Institute of Chemical Engineers National Meeting*. Boston MA, November 2021.
 13. Liu, C.-Y.; **Senftle, T. P.**, “Constructing descriptors in Catalysis with Iterative Bayesian Additive Regression Trees (iBART).” *Ken Kennedy Institute Data Science Conference*. Rice University, October 2021.
 14. Liu, C.-Y.; **Senftle, T. P.**, “Constructing descriptors for metal-support interactions with DFT and statistical learning.” *Machine Learning and Chemical/Materials Science Symposium*. Boston University (Virtual Poster Session), June 2021.
 15. Chen, Y.; **Senftle, T. P.**, “Theoretical insights into PFOA activation over boron nitride.” *American Chemical Society National Meeting*. Virtual, April 2021.
 16. Liu, C.-Y.; **Senftle, T. P.**, “Developing statistical learning tools for understanding metal-support interactions in catalysis.” *American Chemical Society National Meeting*. Virtual, April 2021.
 17. Bhati, M.; **Senftle, T. P.**, “Investigating binder materials for Si anode in Li-ion battery using reactive force fields.” *American Chemical Society National Meeting*. Virtual, April 2021.
 18. Walls, B.; **Senftle, T. P.**, “Theoretical investigation of PFOA oxidation.” *AIChE Southwest Student Regional Conference*. Virtual, March 2021.
→ Awarded first place in *Best Presentation* competition
 19. Liu, C.-Y.; Zhang, S.; Martinez, D.; Li, M.; **Senftle, T. P.**, “Identifying interaction trends between single metal atoms and modified MgO(100) supports with statistical learning.” *American Institute of Chemical Engineers National Meeting*. Virtual, November 2020.
 20. Liu, C.-Y.; Zhang, S.; Martinez, D.; Li, M.; **Senftle, T. P.**, “Exploring Metal-Support Interactions in Catalysis with Statistical Learning.” *American Institute of Chemical Engineers National Meeting*. (Poster) Virtual, November 2020.
 21. Wang, P.; **Senftle, T. P.**, “Selectivity and activity of iron carbide for propane dehydrogenation.” *American Institute of Chemical Engineers National Meeting*. Virtual, November 2020.
 22. Wang, P.; **Senftle, T. P.**, “DFT insights into propane dehydrogenation mechanisms of iron carbide.” *American Institute of Chemical Engineers National Meeting*. (Poster) Virtual, November 2020.
 23. Wang, B.; Duan, L.; Heck, K. N.; Guo, S.; Clark, C.; Arredondo, J.; Wang, M.; **Senftle, T. P.**; Westerhoff, P.; Wen, X.; Song, Y.; Wong, M. S., “Efficient photocatalytic PFOA degradation over boron nitride.” *American Institute of Chemical Engineers National Meeting*. Virtual, November 2020.
 24. Liu, C.-Y.; Zhang, S.; Li, M.; **Senftle, T. P.**, “Investigation of metal adsorption trends on modified MgO supports using density functional theory and statistical learning.” *American Institute of Chemical Engineers National Meeting*. Orlando FL, November, 2019.
 25. Liu, C.-Y.; Zhang, S.; Li, M.; **Senftle, T. P.**, “Physical descriptors for predicting charge transfer at the metal-support interface.” (Poster) *American Institute of Chemical Engineers National Meeting*. Orlando FL, November, 2019.
 26. Clark, C. A., Reddy, C. P.; Xu, H.; Heck, K. N.; Luo, G.; **Senftle, T. P.**; Wong, M. S., “Catalytic Control of Nitrite Reduction Chemistry Towards Ammonia and Hydrazine.” *North American Catalysis Society Meeting*. Chicago, IL, June 2019.
 27. Reddy, P.; Clark, C. A.; Heck, K. N.; Wong, M. S.; **Senftle, T. P.**, “Ab initio investigation of nitrite reduction to ammonia at room temperature through aqueous-phase rhodium catalysis.” (Poster) *Smalley-Curl Institute Research Colloquium*. Houston TX, August, 2019.

28. *Bhati, M.; Senftle, T. P.*, “Multi-scale modeling of Li-ion battery anode materials using reactive force fields.” *American Chemical Society National Meeting*. Orlando FL, April 2019.
→ Selected as Best Presentation in the session “Computers in Chemistry”
29. *Bhati, M.; Senftle, T. P.*, “Multi-scale modeling of Li-ion battery anode materials using reactive force fields.” (Poster) *Rice Oil & Gas HPC Conference*. Houston TX, March 2019.
30. *Reddy, P.*; Clark, C. A.; Heck, K. N.; Wong, M. S.; *Senftle, T. P.*, “Ab initio investigation of nitrite reduction to ammonia and dinitrogen at room temperature through Pd and Rh catalysis.” (Poster) *Southwest Catalysis Society Spring Meeting*. Houston TX, August, 2018.

Research Funding:

Total Support as Lead PI: **\$1,349,083⁺** (External: \$1,274,083; Internal: \$75,000)

Total Senftle Lab Allocation: **\$1,225,835⁺** (External: \$1,165,835; Internal: \$60,000)

1. National Science Foundation: CHE-Chemical Catalysis Program (Award #2247729)
Molecular design of photoactive covalent organic frameworks capable of reductive and oxidative degradation of perfluoroalkyl substances
 - Funding: **\$434,507⁺** (PI, Senftle Lab: **\$220,000⁺**)
 - Duration: 7/1/2023 – 6/30/2026
2. National Science Foundation: CAREER Award, CBET-Catalysis Program (Award #2143941)
CAREER: Understanding metal/support interactions in catalysis with statistical learning
 - Funding: **\$572,110⁺** (PI, Senftle Lab: **\$572,110⁺**)
 - Duration: 7/1/2022 – 6/30/2027
3. Department of the Army: Materiel Command (Cooperative Agreement #W911NF-21-2-01 18)
CLES-EM: Clean, lean, and efficient synthesis of energetic materials
 - Funding: **\$625,000** (Senior Personnel, Senftle Lab: **\$84,791⁺**)
 - Duration: 7/6/2021 – 12/6/2022
4. Rice University: InterDisciplinary Excellence Award (IDEA)
Designing modular photo-reactors for simultaneous nitrate removal and natural gas processing
 - Funding: **\$75,000⁺** (PI, Senftle Lab: **\$35,000⁺**)
 - Duration: 8/1/2020 – 7/31/2022
5. National Science Foundation: ERC— Nanotechnology Enabled Water Treatment Systems (NEWT Center; Award #1449500)
3 Projects supported by the NEWT Center:
Development of earth-abundant, non-PGM electrocatalysts for nitrate reduction (Core Project)
 - Funding: **\$130,998⁺** (PI, Senftle Lab: **\$130,998⁺**)
 - Duration: 8/1/2022 – 7/31/2023
Simulation-guided mechanistic studies to reduce Pt content in Pt-Cu electrocatalysts for nitrate reduction (Seed Project)
 - Funding: **\$26,468⁺** (PI, Senftle Lab: **\$26,468⁺**)
 - Duration: 12/7/2021 – 6/7/2022
BN-based composites and nanostructures for accelerated PFAS degradation (Seed Project)
 - Funding: **\$53, 830** (co-PI, Senftle Lab: **\$21,468⁺**)
 - Duration: 8/15/2020 – 8/15/2021

6. American Chemical Society: Petroleum Research Fund (Award #59759-DNI6)
Modeling the effects of sulfate and phosphate on the performance of iron-based catalysts for propane dehydrogenation
 - Funding: **\$110,000[†]** (PI, Senftle Lab: **\$110,000[†]**)
 - Duration: 9/1/2019 – 8/31/2022
7. Rice University: Energy and Environment Initiative – Creative Ventures
Understanding irreversible Li losses in porous silicon anodes
 - Funding: **\$50,000** (co-PI, Senftle Lab: **\$25,000[†]**)
 - Duration: 7/1/2018 – 6/30/2020

Teaching:

Rice University, Houston, TX

Evaluation Scale: 1 – 5 (**1 = Excellent**)

1. *Instructor – ChBE 519 Atomistic Simulation and Engineering Application* *Spring 2019, 2020, 2022*
 - Course Evaluation – 2019: **1.0**; 2020: **1.5**; 2022: **1.0**
 - Teaching Evaluation – 2019: **1.0**; 2020: **1.0**; 2022: **1.14**
2. *Instructor – ChBE 411 Chemical Engineering Thermodynamics* *Annually Fall 2017 to 2022; Spring 2023*
 - Course Evaluation – 2017: **1.58**; 2018: **1.29**; 2019: **1.48**; 2020: **1.77**; 2021: **1.87**; 2022: **1.62**
 - Teaching Evaluation – 2017: **1.7**; 2018: **1.16**; 2019: **1.57**; 2020: **1.50**; 2021: **1.68**; 2022: **1.48**

The Pennsylvania State University, University Park, PA

1. *Teaching Fellow – CHE 220 Chemical Engineering Thermodynamics* *Fall 2014*
2. *Student Lecturer – CHE 597 Simulation Methods for Engineers* *Spring 2014, 2015*

Service:

Rice University

1. ChBE Graduate Admissions Committee (Committee Chair: 2021-present) *2017-present*
2. ChBE Graduate Recruiting Committee *2019-present*
3. ChBE Seminar Committee *2019-present*
4. Applied Physics Curriculum Committee *2019-present*
5. ChBE Faculty Search Committee *2022-2023*
6. University Graduate Council *2018-2019*
7. ChBE Undergraduate Committee *2017-present*
8. ChBE Graduate Recruiting Committee *2017-present*

Academic Community Leadership

Elected Positions:

1. Director, Southwest Catalysis Society *2021-present*

Journal Editorship:

2. Guest Editor, ACS ES&T Engineering *2023*
Special Issue: Advancing Environmental Research through Computational Modelling

Conference/Meeting Organization and Chairing Duties:

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| 3. American Institute of Chemical Engineers National Meeting. Orlando, FL
Symposium: <i>Hydrocarbon Conversion</i> | 2023 |
| 4. 28 th North American Catalysis Society Meeting. Providence, RI
Symposium: <i>New Methods in Modeling, Simulation and Machine Learning</i> | 2023 |
| 5. Southwest Catalysis Society, Spring Symposium. Houston, TX | 2023 |
| 6. American Institute of Chemical Engineers National Meeting. Phoenix, AZ
Symposium: <i>Hydrocarbon Conversion I: Nonoxidative processes for hydrocarbon conversion</i> | 2022 |
| 7. Southwest Catalysis Society, Spring Symposium. Houston, TX | 2022 |
| 8. American Institute of Chemical Engineers National Meeting. Boston, MA
Topical Conference: <i>Applications of Data Science to Molecules and Materials</i> | 2021 |
| 9. Southwest Catalysis Society, Fall Symposium. Virtual Meeting | 2021 |
| 10. American Institute of Chemical Engineers National Meeting. San Francisco, CA (Virtual)
Topical Conference: <i>Applications of Data Science to Molecules and Materials</i> | 2020 |
| 11. American Institute of Chemical Engineers National Meeting. Orlando, FL
Symposium: <i>Fundamentals of Catalysis: Hydrogenation and Dehydrogenation</i> | 2019 |
| 12. 26 th North American Catalysis Society Meeting. Chicago, IL
Symposium: <i>Modeling and Simulation - Catalysis Fundamentals</i> | 2019 |

Awards and Honors:

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| 1. Teaching + Research Excellence Award, <i>George R. Brown School of Engineering, Rice University</i> | 2023 |
| 2. National Science Foundation CAREER Award, <i>CBET – Catalysis</i> | 2022 |
| 3. Younger Chemist Award, <i>American Chemical Society – Greater Houston Section</i> | 2022 |
| 4. Rice Center for Career Development – Career Champion | 2020 |
| 5. Doctoral New Investigator Award, <i>ACS-Petroleum Research Fund</i> | 2019 |
| 6. UOP-Honeywell Invitational Lecturer | 2019 |
| 7. Kokes Award, <i>24th North American Meeting of the Catalysis Society</i> | 2015 |
| 8. AIChE Best Presentation in <i>Rational Catalyst Design, AIChE Annual Meeting</i> | 2015 |
| 9. Gordon Conference on Catalysis: Gary McVicker Poster Award, <i>Second Place</i> | 2014 |

Students Advised:**Doctoral:**

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| 1. Tafadzwa Mutepaire (ChBE) | 2022-present |
| 2. Chase Sellers (ChBE) | 2021-present |
| 3. Peixuan Jin (ChBE) | 2021-present |
| 4. Yu Chen (ChBE) | 2019-present |
| 5. Peng Wang (ChBE) – Current Position: OpenEye Scientific, Inc.
Doctoral Thesis: <i>“Understanding and Designing Heterogeneous Catalysts with Computational Modeling and Machine Learning”</i> | 2018-2023 |
| 6. Manav Bhati (PhD., ChBE) – Current Position: Schrodinger, Inc.
Doctoral Thesis: <i>“Multiscale Modeling of Electrochemical Interfaces”</i> | 2017-2022 |
| 7. Chun-Yen Liu (PhD., ChBE) – Current Position: AspenTech, Inc.
Doctoral Thesis: <i>“Unraveling Metal-Support Interactions in Catalysis with DFT and Statistical Learning”</i> | 2017-2022 |

Masters:

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| 1. Ai-Shi Wang (MS, ChBE) – Enrolled in PhD program at Rice U. | 2021-2023 |
| Masters Thesis: <i>“DFT Investigation of PFAS Adsorption Configurations on Metal Surfaces”</i> | |
| 2. Prakash Chintakunta (MS, Applied Physics) | 2017-2020 |
| Masters Thesis: <i>“Elucidating Aqueous Nitrite Reduction Mechanisms on Pd and Rh Catalysts”</i> | |

Undergraduate:

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| 1. Jenna Parrott (Civil E, Lone Star College) | 2023-present |
| 2. Samuel Nance (ChBE) | 2023-present |
| 3. Benjamin Walls (BS, ChBE) – NSF GRFP Recipient, Enrolled in PhD program at U. of Michigan | 2020-2023 |
| 4. Vania Ding (BS, ChBE) | 2020 |
| 5. Daniel Martinez (BS, ChBE) | 2018-2020 |
| 6. Jonathan Chapman (BS, ChBE) | 2018-2019 |
| 7. Burk Garza (BS, ChBE) – Enrolled in PhD program at U. of Pittsburgh | 2018 |

Major Awards and Honors for Advised Students:

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|---|------|
| 1. National Science Foundation GRFP, <i>Ben Walls</i> | 2023 |
| 2. American Society of Indian Engineers and Architects (ASIE) Scholarship, <i>Manav Bhati</i> | 2021 |
| 3. Daxin Materials Corporation Fellowship, <i>Chun-Yen Liu</i> | 2021 |
| 4. Riki Kobayashi Fellowship, <i>Manav Bhati</i> | 2020 |
| 5. Ken Kennedy Institute Graduate Fellowship, <i>Manav Bhati</i> | 2019 |