

Yulun Han

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Education

- 2013–2015 Ph.D., Materials Chemistry, University of South Dakota
Thesis Title: The Photofragmentation Mechanisms of Gas-phase Rare Earth Complexes for Laser-Assisted Metal-Organic Chemical Vapor Deposition: Isopropylcyclopentadienyl and Trimethylsilylamido Ligand Examples
Advisor: Mary T. Berry
- 2010–2013 M.Sc., Chemistry, University of South Dakota
Thesis Title: Crystallographic Models for the Coordination Geometry and Electronic Relaxation Mechanisms of Ln^{3+} Complexes in the Ionic Liquid BMICl
Advisor: Mary T. Berry
- 2005–2009 B.Sc., Applied Chemistry, Donghua University

Appointments

- 2024– Assistant Professor, Texas A&M University-San Antonio
- 2018–2024 Postdoctoral Researcher, North Dakota State University
- 2016–2018 Visiting Scholar, North Dakota State University
- 2015–2016 Postdoctoral Researcher, University of South Dakota
- 2010–2015 Graduate Research Assistant, University of South Dakota

Honours and Awards

- 2025 Texas A&M University-San Antonio Research Council Grant
- 2018 Sanibel Symposium Löwdin Postdoc Award

Teaching

FA2026	Physical Chemistry I	Texas A&M University-San Antonio
FA2026	Physical Chemistry I Laboratory	Texas A&M University-San Antonio
FA2026	General Chemistry I Laboratory	Texas A&M University-San Antonio
SP2026	General Chemistry II	Texas A&M University-San Antonio
SP2026	General Chemistry II Recitation	Texas A&M University-San Antonio
SP2026	General Chemistry II Laboratory	Texas A&M University-San Antonio
FA2025	Physical Chemistry I	Texas A&M University-San Antonio
FA2025	Physical Chemistry I Laboratory	Texas A&M University-San Antonio
FA2025	General Chemistry I	Texas A&M University-San Antonio
FA2025	General Chemistry I Recitation	Texas A&M University-San Antonio
SP2025	General Chemistry I	Texas A&M University-San Antonio
SP2025	General Chemistry I Laboratory	Texas A&M University-San Antonio
SP2025	General Chemistry II Laboratory	Texas A&M University-San Antonio
FA2024	Inorganic Chemistry	Texas A&M University-San Antonio
FA2024	Inorganic Chemistry Laboratory	Texas A&M University-San Antonio

Publications

Journals

- [1] **Han, Y.**; Micha, D. A.; Kilin, D. S. First-Principles Calculations and Machine Learning for Nonradiative Relaxation of Charge Carriers at Nanostructured Ag₃Si(111) Monolayered Surfaces. *The Journal of Physical Chemistry Letters* 2026, 17 (28), 8032-8037. DOI: [10.1021/acs.jpcllett.6c01516](https://doi.org/10.1021/acs.jpcllett.6c01516)
- [2] Raju, M. M. K.; **Han, Y.**; Kilin, D.; Ding, Y.; Zhang, Q. Toward an Improved Solid-State Li Electrolyte: A First-Principles Investigation of the Structure, Li-Ion Migration Pathways, and Ionic Conductivity of Li₇La₃Zr₂O₁₂. *European Journal of Chemistry* 2026, 17 (2), 125-137. DOI: [10.5155/eurjchem.17.2.125-137.2759](https://doi.org/10.5155/eurjchem.17.2.125-137.2759)
- [3] Thapa, D.; **Han, Y.**; Weight, B. M.; Tiffany, G.; Kilin, D.; Tretiak, S.; Kilina, S. Singlet and Triplet Excitations in Chemically Functionalized Single-Walled Carbon Nanotubes. *Journal of Materials Chemistry C* 2026, 14 (11), 4482-4495. DOI: [10.1039/d5tc03222a](https://doi.org/10.1039/d5tc03222a)
- [4] Ghazanfari, S.; **Han, Y.**; Arshad, A.; Xia, W.; Kilina, S.; Kilin, D. Exploring Peptide Bond Formation Using Transition State Search and Wave Packet Dynamics. *The Journal of Physical Chemistry Letters* 2025, 16 (27), 6968-6974. DOI: [10.1021/acs.jpcllett.5c01096](https://doi.org/10.1021/acs.jpcllett.5c01096)

- [5] **Han, Y.**; Vazhappilly, T.; Micha, D. A.; Kilin, D. S. Relaxation of Photoexcited Electron–Hole Pairs at Si(111) Surfaces with Adsorbed Ag Monolayered Clusters of Increasing Size. *The Journal of Physical Chemistry Letters* 2025, 16 (11), 2905–2913. DOI: [10.1021/acs.jpcllett.4c03735](https://doi.org/10.1021/acs.jpcllett.4c03735)
- [6] Qu, H.; **Han, Y.**; Fortner, J.; Wu, X.; Kilina, S.; Kilin, D.; Tretiak, S.; Wang, Y. [2 + 2] Cycloaddition Produces Divalent Organic Color-Centers with Reduced Heterogeneity in Single-Walled Carbon Nanotubes. *Journal of the American Chemical Society* 2024, 146 (33), 23582–23590. DOI: [10.1021/jacs.4c08105](https://doi.org/10.1021/jacs.4c08105)
- [7] Liu, B.; Wang, Z.; Huang, S.; **Han, Y.**; Kilin, D. S. Effects of Surface Defects on Performance and Dynamics of CsPbI₂Br Perovskite: First-Principles Nonadiabatic Molecular Dynamics Simulations. *The Journal of Physical Chemistry Letters* 2024, 15 (18), 4782–4791. DOI: [10.1021/acs.jpcllett.4c00675](https://doi.org/10.1021/acs.jpcllett.4c00675)
- [8] Keya, K. N.; **Han, Y.**; Xia, W.; Kilin, D. Inter-Oligomer Interaction Influence on Photoluminescence in Cis-Polyacetylene Semiconductor Materials. *Polymers* 2024, 16 (13), 1896. DOI: [10.3390/polym16131896](https://doi.org/10.3390/polym16131896)
- [9] Erickson, M.; Casañola-Martin, G.; **Han, Y.**; Rasulev, B.; Kilin, D. Relationships between the Photodegradation Reaction Rate and Structural Properties of Polymer Systems. *The Journal of Physical Chemistry B* 2024, 128 (9), 2190–2200. DOI: [10.1021/acs.jpcc.3c06854](https://doi.org/10.1021/acs.jpcc.3c06854)
- [10] Inerbaev, T. M.; **Han, Y.**; Bekker, T. B.; Kilin, D. S. Photoluminescence in Cerium-Doped Fluoride Borate Crystals. *The Journal of Physical Chemistry C* 2023, 127 (19), 9213–9224. DOI: [10.1021/acs.jpcc.2c08711](https://doi.org/10.1021/acs.jpcc.2c08711)
- [11] **Han, Y.**; Kilin, D. Photoreactions Create Superconducting Materials. *Journal of Applied Spectroscopy* 2023, 90 (3), 639–645. DOI: [10.1007/s10812-023-01577-9](https://doi.org/10.1007/s10812-023-01577-9)
- [12] Zheng, Y.; **Han, Y.**; Weight, B. M.; Lin, Z.; Gifford, B. J.; Zheng, M.; Kilin, D.; Kilina, S.; Doorn, S. K.; Htoon, H.; Tretiak, S. Photochemical Spin-State Control of Binding Configuration for Tailoring Organic Color Center Emission in Carbon Nanotubes. *Nature Communications* 2022, 13 (1). DOI: [10.1038/s41467-022-31921-0](https://doi.org/10.1038/s41467-022-31921-0)
- [13] Vazhappilly, T.; **Han, Y.**; Kilin, D. S.; Micha, D. A. Electronic Relaxation of Photoexcited Open and Closed Shell Adsorbates on Semiconductors: Ag and Ag₂ on TiO₂. *The Journal of Chemical Physics* 2022, 156 (10). DOI: [10.1063/5.0082748](https://doi.org/10.1063/5.0082748)
- [14] Ghazanfari, S.; **Han, Y.**; Xia, W.; Kilin, D. S. First-Principles Study on Optoelectronic Properties of Fe-Doped Montmorillonite Clay. *The Journal of Physical Chemistry Letters* 2022, 4257–4262. DOI: [10.1021/acs.jpcllett.2c00697](https://doi.org/10.1021/acs.jpcllett.2c00697)
- [15] Erickson, M.; **Han, Y.**; Rasulev, B.; Kilin, D. Molecular Dynamics Study of the Photodegradation of Polymeric Chains. *The Journal of Physical Chemistry Letters* 2022, 4374–4380. DOI: [10.1021/acs.jpcllett.2c00802](https://doi.org/10.1021/acs.jpcllett.2c00802)
- [16] Inerbaev, T. M.; **Han, Y.**; Bekker, T. B.; Kilin, D. S. Mechanisms of Photoluminescence in Copper-Containing Fluoride Borate Crystals. *The Journal of Physical Chemistry C* 2022, 126 (14), 6119–6128. DOI: [10.1021/acs.jpcc.1c10206](https://doi.org/10.1021/acs.jpcc.1c10206)

- [17] Pan, Y.; Li, H.; Lenertz, M.; **Han, Y.**; Ugrinov, A.; Kilin, D.; Chen, B.; Yang, Z. One-Pot Synthesis of Enzyme@metal–Organic Material (MOM) Biocomposites for Enzyme Biocatalysis. *Green Chemistry* 2021. DOI: [10.1039/d1gc00775k](https://doi.org/10.1039/d1gc00775k)
- [18] **Han, Y.**; Iduoku, K.; Grant, G.; Rasulev, B.; Leontyev, A.; Hobbie, E. K.; Tretiak, S.; Kilina, S. V.; Kilin, D. S. Hot Carrier Dynamics at Ligated Silicon(111) Surfaces: A Computational Study. *The Journal of Physical Chemistry Letters* 2021, 7504–7511. DOI: [10.1021/acs.jpcclett.1c02084](https://doi.org/10.1021/acs.jpcclett.1c02084)
- [19] Pringle, T. A.; Hunter, K. I.; Brumberg, A.; Anderson, K. J.; Fagan, J. A.; Thomas, S. A.; Petersen, R. J.; Sefannaser, M.; **Han, Y.**; Brown, S. L.; Kilin, D. S.; Schaller, R. D.; Kortshagen, U. R.; Boudjouk, P. R.; Hobbie, E. K. Bright Silicon Nanocrystals from a Liquid Precursor: Quasi-Direct Recombination with High Quantum Yield. *ACS Nano* 2020, 14 (4), 3858–3867. DOI: [10.1021/acsnano.9b09614](https://doi.org/10.1021/acsnano.9b09614)
- [20] **Han, Y.**; Kilin, D. S. Nonradiative Relaxation Dynamics of a Cesium Lead Halide Perovskite Photovoltaic Architecture: Effect of External Electric Fields. *The Journal of Physical Chemistry Letters* 2020, 11 (23), 9983–9989. DOI: [10.1021/acs.jpcclett.0c02973](https://doi.org/10.1021/acs.jpcclett.0c02973)
- [21] Fatima; **Han, Y.**; Vogel, D. J.; Inerbaev, T. M.; Oncel, N.; Hobbie, E. K.; Kilin, D. S. Photoexcited Electron Lifetimes Influenced by Momentum Dispersion in Silicon Nanowires. *The Journal of Physical Chemistry C* 2019, 123 (12), 7457–7466. DOI: [10.1021/acs.jpcc.9b00639](https://doi.org/10.1021/acs.jpcc.9b00639)
- [22] Nayakasinghe, M. T.; **Han, Y.**; Sivapragasam, N.; Kilin, D. S.; Oncel, N.; Burghaus, U. Adsorption of Formic Acid on $\text{CH}_3\text{NH}_3\text{PbI}_3$ Lead–Halide Organic–Inorganic Perovskites. *The Journal of Physical Chemistry C* 2019, 123 (37), 22873–22886. DOI: [10.1021/acs.jpcc.9b03319](https://doi.org/10.1021/acs.jpcc.9b03319)
- [23] **Han, Y.**; Hobbie, E. K.; Kilin, D. S. First-Principles Molecular Dynamics of Monomethylhydrazine and Nitrogen Dioxide. *The Journal of Physical Chemistry Letters* 2019, 10 (10), 2394–2399. DOI: [10.1021/acs.jpcclett.9b00674](https://doi.org/10.1021/acs.jpcclett.9b00674)
- [24] Fatima; Vogel, D. J.; **Han, Y.**; Inerbaev, T. M.; Oncel, N.; Kilin, D. S. First-Principles Study of Electron Dynamics with Explicit Treatment of Momentum Dispersion on Si Nanowires along Different Directions. *Molecular Physics* 2018, 117 (17), 2293–2302. DOI: [10.1080/00268976.2018.1538624](https://doi.org/10.1080/00268976.2018.1538624)
- [25] Disrud, B.; **Han, Y.**; Gifford, B. J.; Kilin, D. S. Molecular Dynamics of Reactions between (4,0) Zigzag Carbon Nanotube and Hydrogen Peroxide under Extreme Conditions. *Molecular Physics* 2018, 116 (5–6), 708–716. DOI: [10.1080/00268976.2017.1420258](https://doi.org/10.1080/00268976.2017.1420258)
- [26] **Han, Y.**; Anderson, K.; Hobbie, E. K.; Boudjouk, P.; Kilin, D. S. Unraveling Photodimerization of Cyclohexasilane from Molecular Dynamics Studies. *The Journal of Physical Chemistry Letters* 2018, 9 (15), 4349–4354. DOI: [10.1021/acs.jpcclett.8b01691](https://doi.org/10.1021/acs.jpcclett.8b01691)
- [27] Nayakasinghe, M. T.; **Han, Y.**; Sivapragasam, N.; Kilin, D. S.; Burghaus, U. Unexpected High Binding Energy of CO_2 on $\text{CH}_3\text{NH}_3\text{PbI}_3$ Lead-Halide Organic–Inorganic Perovskites via Bicarbonate Formation. *Chemical Communications* 2018. DOI: [10.1039/c8cc04749a](https://doi.org/10.1039/c8cc04749a)

- [28] Disrud, B.; **Han, Y.**; Kilin, D. S. Molecular Dynamics of Laser-Assisted Decomposition of Unstable Molecules at the Surface of Carbon Nanotubes: Case Study of $\text{CH}_2(\text{NO}_2)_2$ on CNT(4,0). *Molecular Physics* 2017, 115 (5), 674–682. DOI: [10.1080/00268976.2017.1290838](https://doi.org/10.1080/00268976.2017.1290838)
- [29] **Han, Y.**; Rasulev, B.; Kilin, D. S. Photofragmentation of Tetranitromethane: Spin-Unrestricted Time-Dependent Excited-State Molecular Dynamics. *The Journal of Physical Chemistry Letters* 2017, 8 (14), 3185–3192. DOI: [10.1021/acs.jpcllett.7b01330](https://doi.org/10.1021/acs.jpcllett.7b01330)
- [30] **Han, Y.**; Meng, Q.; Rasulev, B.; May, P. S.; Berry, M. T.; Kilin, D. S. Photoinduced Charge Transfer versus Fragmentation Pathways in Lanthanum Cyclopentadienyl Complexes. *Journal of Chemical Theory and Computation* 2017, 13 (9), 4281–4296. DOI: [10.1021/acs.jctc.7b00050](https://doi.org/10.1021/acs.jctc.7b00050)
- [31] **Han, Y.**; Vogel, D. J.; Inerbaev, T. M.; May, P. S.; Berry, M. T.; Kilin, D. S. Photoinduced Dynamics to Photoluminescence in Ln^{3+} ($\text{Ln} = \text{Ce}, \text{Pr}$) Doped $\beta\text{-NaYF}_4$ Nanocrystals Computed in Basis of Non-Collinear Spin DFT with Spin-Orbit Coupling. *Molecular Physics* 2017, 116 (5–6), 697–707. DOI: [10.1080/00268976.2017.1416193](https://doi.org/10.1080/00268976.2017.1416193)
- [32] Hogoboom, D.; **Han, Y.**; Kilin, D. A Computational Study of the Combustion of Hydrazine with Dinitrogen Tetroxide. *Journal of Nanotoxicology and Nanomedicine* 2017, 2 (2), 12–30. DOI: [10.4018/jnn.2017070102](https://doi.org/10.4018/jnn.2017070102)
- [33] **Han, Y.**; Kilin, D. S.; May, P. S.; Berry, M. T.; Meng, Q. Photofragmentation Pathways for Gas-Phase Lanthanide Tris(Isopropylcyclopentadienyl) Complexes. *Organometallics* 2016, 35 (20), 3461–3473. DOI: [10.1021/acs.organomet.6b00420](https://doi.org/10.1021/acs.organomet.6b00420)
- [34] Junkman, D.; Vogel, D. J.; **Han, Y.**; Kilin, D. S. Ab Initio Analysis of Charge Carrier Dynamics in Organic-Inorganic Lead Halide Perovskite Solar Cells. *MRS Proceedings* 2015, 1776, 19–29. DOI: [10.1557/opl.2015.782](https://doi.org/10.1557/opl.2015.782)
- [35] **Han, Y.**; Meng, Q.; Rasulev, B.; May, P. S.; Berry, M. T.; Kilin, D. S. Photofragmentation of the Gas-Phase Lanthanum Isopropylcyclopentadienyl Complex: Computational Modeling vs Experiment. *The Journal of Physical Chemistry A* 2015, 119 (44), 10838–10848. DOI: [10.1021/acs.jpca.5b07209](https://doi.org/10.1021/acs.jpca.5b07209)
- [36] **Han, Y.**; Micha, D. A.; Kilin, D. S. Ab Initio study of the Photocurrent at the Au/Si Metal–Semiconductor Nanointerface. *Molecular Physics* 2014, 113 (3–4), 327–335. DOI: [10.1080/00268976.2014.944598](https://doi.org/10.1080/00268976.2014.944598)
- [37] **Han, Y.**; Lin, C.; Meng, Q.; Dai, F.; Sykes, A. G.; Berry, M. T.; May, P. S. $(\text{BMI})_3\text{LnCl}_6$ Crystals as Models for the Coordination Environment of LnCl_3 ($\text{Ln} = \text{Sm}, \text{Eu}, \text{Dy}, \text{Er}, \text{Yb}$) in 1-Butyl-3-Methylimidazolium Chloride Ionic-Liquid Solution. *Inorganic Chemistry* 2014, 53 (11), 5494–5501. DOI: [10.1021/ic500101x](https://doi.org/10.1021/ic500101x)
- [38] **Han, Y.**; Tretiak, S.; Kilin, D. Dynamics of Charge Transfer at Au/Si Metal–Semiconductor Nano-Interface. *Molecular Physics* 2013, 112 (3–4), 474–484. DOI: [10.1080/00268976.2013.842007](https://doi.org/10.1080/00268976.2013.842007)
- [39] **Han, Y.**; Dai, F.; Sykes, A. G.; May, P. S.; Berry, M. T.; Meng, Q.; Lin, C. Catena-Poly[1-Butyl-3-Methylimidazolium [[Dichlorido(Methanol- κO)(Propan-2-Ol- κO)Lanthanate(III)]-Di- μ -Chlorido]]. *Acta Crystallographica Section E Structure Reports Online* 2012, 68 (3), m292–m293. DOI: [10.1107/s160053681200517x](https://doi.org/10.1107/s160053681200517x)

Book

- [1] Kilin, D., Kilina, S.V. and **Han, Y.** (eds) (2019) Computational photocatalysis: modeling of photophysics and photochemistry at interfaces. Washington, DC : American Chemical Society. Available at: <http://dx.doi.org/10.1021/bk-2019-1331>.

Contributed Presentations

- [1] **Han, Y.** Relaxation of photoexcited electron-hole pairs at nanostructured Si(111) surfaces from quantum dissipative dynamics and machine learning (oral presentation), Computational Photocatalysis: Photophysics & Photochemistry at Interfaces. Machine Learning Bridges Theory and Experiment (Symposium CTH005), Pacificchem 2025, Honolulu, HI, December 2025.
- [2] **Han, Y.** Study of Chemical Reactions via ab initio Molecular Dynamics (oral presentation), Modeling exciton and charge dynamics in molecules and clusters toward optoelectronic applications (Symposium 201), Pacificchem 2020, Virtual, December 2021.
- [3] **Han, Y.** Time-dependent Excited-state Molecular Dynamics: from Photofragmentation to Photopolymerization (oral presentation), Physics Seminar, North Dakota State University, Fargo, ND, February 2018.
- [4] **Han, Y.** Photofragmentation of Tetranitromethane: Spin-unrestricted Time-dependent Excited-state Molecular Dynamics (oral presentation), American Chemical Society (ACS) Great Lakes Regional Meeting: Photophysics & Photochemistry of Interfaces, Fargo, ND, June 2017.
- [5] **Han, Y.** One Dimensional Conducting Polymer Nanocomposites (oral presentation), Department of Chemistry Seminar, University of South Dakota, Vermillion, SD, April 2011.

Professional Activities

- Event Coordinator, Materials Science, San Antonio Regional Science Olympiad, 2025–2026
- Faculty Advisor, Jaguar Chemistry Club, Texas A&M University-San Antonio, 2024–2026
- Session Chair, "ML for Photophysics", Computational Photocatalysis: Photophysics & Photochemistry at Interfaces. Machine Learning Bridges Theory and Experiment (Symposium CTH005), Pacificchem 2025, 2025
- Session Chair, "Quantum Dynamics of Molecular Interactions and Materials", 64th Sanibel Symposium, 2025
- Panelist, Research Computing Needs and Use Cases, Texas A&M University-San Antonio, 2025

- Organizer, "Computational Photocatalysis: Modeling Photophysics and Photochemistry at Interfaces" Symposium, 256th ACS National Meeting & Exposition, 2018
- Committee Member, Distinguished Student Award Committee of the Department of Natural Sciences, Texas A&M University-San Antonio, 2025
- Committee Member, Laboratory Chemical and Physical Safety Committee, Texas A&M University-San Antonio, 2024
- Committee Member, Assistant Professor of Inorganic Chemistry Search Committee Texas A&M University-San Antonio, 2024
- Committee Member, Assistant Professor of Analytical Chemistry Search Committee, Texas A&M University-San Antonio, 2024
- Reviewer, Texas A&M University-San Antonio Research Council Grant, 2026
- Reviewer, ACS Nano, 2025
- Reviewer, RSC Advance, 2024
- Reviewer, Materials Letters, 2017–2018
- Reviewer, Journal of Alloys and Compounds, 2018
- Reviewer, Nanotechnology, 2018
- Reviewer, Materials Research Bulletin, 2017–2021
- Reviewer, Materials Science and Engineering: B, 2017