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RESEARCH EXPERIENCE AND APPOINTMENTS

09/2024-present Assistant Professor, Texas A&M University-San Antonio, San Antonio, TX
04/2018-08/2024 Postdoctoral Researcher, North Dakota State University, Fargo, ND
09/2016-04/2018 Visiting Scholar, North Dakota State University, Fargo, ND
08/2015-07/2016 Postdoctoral Researcher, University of South Dakota, Vermillion, SD
09/2010–08/2015 Graduate Research Assistant, University of South Dakota, Vermillion, SD

EDUCATION

05/2013-08/2015 Ph.D. in Materials Chemistry, University of South Dakota, Vermillion, SD
Advisor: Prof. Mary T. Berry
Thesis title: *The Photofragmentation Mechanisms of Gas-phase Rare Earth Complexes for Laser-Assisted Metal-Organic Chemical Vapor Deposition: Isopropylcyclopentadienyl and Trimethylsilylamido Ligand Examples*
08/2010-05/2013 M.S. in Chemistry, University of South Dakota, Vermillion, SD
Advisor: Prof. Mary T. Berry
Thesis title: *Crystallographic Models for the Coordination Geometry and Electronic Relaxation Mechanisms of Ln³⁺ Complexes in the Ionic Liquid BMICl*
09/2005-07/2009 B.S. in Applied Chemistry, Donghua University, Shanghai, China

TEACHING

09/2024-present Inorganic Chemistry (CHEM 4390), Inorganic Chemistry Laboratory (CHEM 4190), Texas A&M University-San Antonio, San Antonio, TX

PUBLICATIONS

Journal articles (*corresponding author)

1. H. Qu, **Y. Han**, J. Fortner, X. Wu, S. Kilina, D. Kilin, S. Tretiak, Y. Wang. [2+ 2] Cycloaddition Produces Divalent Organic Color-Centers with Reduced Heterogeneity in Single-Walled Carbon Nanotubes. *J. Am. Chem. Soc.* 2024, 146, 33, 23582–23590

2. K. N. Keya, **Y. Han**, W. Xia, D. Kilin. Inter-Oligomer Interaction Influence on Photoluminescence in Cis-Polyacetylene Semiconductor Materials. *Polymers* 2024, 16, 13, 1896.
3. B. Liu, Z. Wang, S. Huang, **Y. Han***, D. S. Kilin. Effects of Surface Defects on Performance and Dynamics of CsPbI₂Br Perovskite: First-Principles Nonadiabatic Molecular Dynamics Simulations. *J. Phys. Chem. Lett.* 2024, 15, 18, 4782–4791.
4. M. Erickson, G. Casañola-Martin, **Y. Han**, B. Rasulev, D. Kilin. Relationships Between Photo-degradation Reaction Rate and Structural Properties of Polymer Systems. *J. Phys. Chem. B* 2024, 128, 9, 2190–2200.
5. **Y. Han**, D. Kilin. Photoreactions Create Superconducting Materials. *J. Appl. Spectrosc.* 2023, 90, 639–645.
6. T. M. Inerbaev, **Y. Han**, T. B. Bekker, and D. S. Kilin. Photoluminescence in Cerium-Doped Fluoride Borate Crystals. *J. Phys. Chem. C.* 2023, 127, 19, 9213-9224.
7. Y. Zheng, **Y. Han**, B. M. Weight, Z. Lin, B. J. Gifford, M. Zheng, D. Kilin, S. Kilina, S. K. Doorn, H. Htoon, S. Tretiak. Photochemical Spin-State Control of Binding Configuration for Tailoring Organic Color Center Emission in Carbon Nanotubes. *Nat. Commun.* 2022, 13, 4439.
8. M. Erickson, **Y. Han**, B. Rasulev, D. Kilin. Molecular Dynamics Study of the Photodegradation of Polymeric Chains. *J. Phys. Chem. Lett.* 2022, 13, 19, 4374-4380.
9. S. Ghazanfari, **Y. Han**, W. Xia, D. S. Kilin. First-Principles Study on Optoelectronic Properties of Fe-Doped Montmorillonite Clay. *J. Phys. Chem. Lett.* 2022, 13, 19, 4257-4262.
10. T. M. Inerbaev, **Y. Han**, T. B. Bekker, D. S. Kilin. Mechanisms of Photoluminescence in Cu-Containing Fluoride Borate Crystals. *J. Phys. Chem. C.* 2022, 126, 14, 6119-6128.
11. T. Vazhappilly, **Y. Han**, D. S. Kilin, D. A. Micha. Electronic Relaxation of Photoexcited Open and Closed Shell Adsorbates on Semiconductors: Ag and Ag₂ on TiO₂. *J. Chem. Phys.* 2022, 156, 10, 104705.
12. **Y. Han**, K. Iduoku, G. Grant, B. Rasulev, A. Leontyev, E. K. Hobbie, S. Tretiak, S. V. Kilina, D. S. Kilin. Hot Carrier Dynamics at Ligated Silicon (111) Surfaces: A Computational Study. *J. Phys. Chem. Lett.* 2021, 12, 31, 7504–7511.
13. Y. Pan, H. Li, M. Lenertz, **Y. Han**, A. Ugrinov, D. Kilin, B. Chen, Z. Yang. One-pot Synthesis of Enzyme@Metal–Organic Material (MOM) Biocomposites for Enzyme Biocatalysis. *Green Chem.* 2021, 23, 4466-4476.
14. **Y. Han**, D. S. Kilin. Nonradiative Relaxation Dynamics of a Cesium Lead Halide Perovskite Photovoltaic Architecture: Effect of External Electric Fields. *J. Phys. Chem. Lett.* 2020, 11, 23, 9983-9989.
15. T. A. Pringle, K. I. Hunter, A. Brumberg, K. J. Anderson, J. A. Fagan, S. A. Thomas, R. J. Petersen, M. Sefannaser, **Y. Han**, S. L. Brown, D. S. Kilin, R. D. Schaller, U. R. Kortshagen, P. R. Boudjouk, E. K. Hobbie. Bright Silicon Nanocrystals from a Liquid Precursor: Quasi-Direct Recombination with High Quantum Yield. *ACS Nano* 2020, 14, 4, 3858-3867.

16. M. T. Nayakasinghe, **Y. Han**, N. Sivapragasam, D. S. Kilin, N. Oncel, U. Burghaus. Adsorption of Formic Acid on $\text{CH}_3\text{NH}_3\text{PbI}_3$ Lead-Halide Organic-Inorganic Perovskites. *J. Phys. Chem. C* 2019, 123, 37, 22873-22886.
17. Fatima, D. J Vogel, **Y. Han**, T. M. Inerbaev, N. Oncel, D. S. Kilin. First-principles Study of Electron Dynamics with Explicit Treatment of Momentum Dispersion on Si Nanowires along Different Directions. *Mol. Phys.* 2019, 117, 17, 2293-2302.
18. **Y. Han**, E. K. Hobbie, D. S. Kilin. First-Principles Molecular Dynamics of Monomethylhydrazine and Nitrogen Dioxide. *J. Phys. Chem. Lett.* 2019, 10, 10, 2394-2399.
19. Fatima, **Y. Han**, D. J. Vogel, T. M. Inerbaev, N. Oncel, E. K. Hobbie, D. S. Kilin. Photoexcited Electron Lifetimes Influenced by Momentum Dispersion in Silicon Nanowires. *J. Phys. Chem. C* 2019, 123, 12, 7457-7466.
20. **Y. Han**, K. Anderson, E. K. Hobbie, P. Boudjouk, D. S. Kilin. Unraveling Photodimerization of Cyclohexasilane from Molecular Dynamics Studies. *J. Phys. Chem. Lett.* 2018, 9, 15, 4349-4354.
21. M. T. Nayakasinghe, **Y. Han**, N. Sivapragasam, D. S. Kilin, U. Burghaus. 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. *Chem. Comm.* 2018, 54, 71, 9949-9952.
22. B. Disrud, **Y. Han**, B. J Gifford, D. S. Kilin. Molecular Dynamics of Reactions between (4,0) Zigzag Carbon Nanotube and Hydrogen Peroxide under Extreme Conditions. *Mol. Phys.* 2018, 116, 5-6, 708-716.
23. **Y. Han**, D. J. Vogel, T. M. Inerbaev, P. S. May, M. T. Berry, D. S. Kilin. 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. *Mol. Phys.* 2018, 116, 5-6, 697-707.
24. D. Hogoboom, **Y. Han**, D. Kilin. A Computational Study of the Combustion of Hydrazine with Dinitrogen Tetroxide. *Journal of Nanotoxicology and Nanomedicine (JNN)* 2017, 2, 2, 12-30.
25. **Y. Han**, Q. Meng, B. Rasulev, P. S. May, M. T. Berry, D. S. Kilin. Photoinduced Charge Transfer versus Fragmentation Pathways in Lanthanum Cyclopentadienyl Complexes. *J. Chem. Theory Comput.* 2017, 13, 9, 4281-4296.
26. **Y. Han**, B. Rasulev, D. S. Kilin. Photofragmentation of Tetranitromethane: Spin-Unrestricted Time-Dependent Excited-State Molecular Dynamics. *J. Phys. Chem. Lett.* 2017, 8, 14, 3185-3192.
27. B. Disrud, **Y. Han**, D. S. Kilin. 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 $\text{CNT}(4,0)$. *Mol. Phys.* 2017, 115, 5, 674-682.
28. **Y. Han**, D. S. Kilin, P. S. May, M. T. Berry, Q. Meng. Photofragmentation Pathways for Gas-Phase Lanthanide Tris(isopropylcyclopentadienyl) Complexes. *Organometallics* 2016, 35, 20, 3461-3473.

29. **Y. Han**, Q. Meng, B. Rasulev, P. S. May, M. T. Berry, D. S. Kilin. Photofragmentation of the Gas-Phase Lanthanum Isopropylcyclopentadienyl Complex: Computational Modeling Vs Experiment. *J. Phys. Chem. A* 2015, 119, 44, 10838-10848.
30. D. Junkman, D. J. Vogel, **Y. Han**, D. S. Kilin. Ab Initio Analysis of Charge Carrier Dynamics in Organic-Inorganic Lead Halide Perovskite Solar Cells. *MRS Online Proc. Libr.* 2015, 1776, 19-29.
31. **Y. Han**, D. A. Micha, D. S. Kilin. Ab initio Study of the Photocurrent at the Au/Si Metal-semiconductor Nanointerface. *Mol. Phys.* 2015, 113, 3-4, 327-335.
32. **Y. Han**, C. Lin, Q. Meng, F. Dai, A. G. Sykes, M. T. Berry, P. S. May. (BMI)₃LnCl₆ Crystals as Models for the Coordination Environment of LnCl₃ (Ln = Sm, Eu, Dy, Er, Yb) in 1-Butyl-3-methylimidazolium Chloride Ionic-Liquid Solution. *Inorganic Chem.* 2014, 53, 11, 5494-5501.
33. **Y. Han**, S. Tretiak, D. Kilin. Dynamics of Charge Transfer at Au/Si Metal-semiconductor Nano-interface. *Mol. Phys.* 2014, 112, 3-4, 474-484.
34. **Y. Han**, F. Dai, A. G. Sykes, P. S. May, M. T. Berry, Q. Meng, C. Lin. catena-Poly[1-butyl-3-methyl-imidazolium[[dichlorido(methanol-κO)(propan-2-ol-κO)lanthanate(III)]-di-μ-chlorido]]. *Acta Crystallogr., Sect. E: Crystallogr. Commun.* 2012, 68, 3, m292-m293.

Book

D. Kilin; S. Kilina; **Y. Han**. Computational Photocatalysis: Modeling Photophysics and Photochemistry at Interfaces. ACS Symposium Series, Volume 1331, ISBN 9780841235540, American Chemical Society: Washington DC.

PRESENTATIONS

Invited talks

- 12/2021 “Study of chemical reactions via ab initio molecular dynamics”, Pacificchem 2021, Symposium 201 (virtual): Modeling exciton and charge dynamics in molecules and clusters toward optoelectronic applications.
- 02/2018 “Time-dependent Excited-state Molecular Dynamics: from Photofragmentation to Photopolymerization”, Physics Seminar, North Dakota State University, Fargo, ND.
- 06/2017 “Photofragmentation of Tetranitromethane: Spin-unrestricted Time-dependent Excited-state Molecular Dynamics”, American Chemical Society (ACS) Great Lakes Regional Meeting: Photophysics & Photochemistry of Interfaces, Fargo, ND.
- 04/2011 “One Dimensional Conducting Polymer Nanocomposites”, Department of Chemistry Seminar, University of South Dakota, Vermillion, SD.

Posters

- 10/2023 Conference on Computational Science, Fargo, ND
- 02/2023 62nd Sanibel Symposium, St. Simons Island, GA

02/2022	61 st Sanibel Symposium, St. Simons Island, GA
02/2020	60 th Sanibel Symposium, St. Simons Island, GA
02/2019	59 th Sanibel Symposium, St. Simons Island, GA
08/2018	256 th ACS National Meeting, Boston, MA
06/2018	Excited State Processes in Electronic and Bio Nanomaterials, Santa Fe, NM
02/2018	58 th Sanibel Symposium, St. Simons Island, GA
10/2017	NDSU-KU Joint Symposium, Fargo, ND
02/2017	57 th Sanibel Symposium, St. Simons Island, GA
08/2016	252 nd ACS National Meeting, Philadelphia, PA
02/2016	56 th Sanibel Symposium, St. Simons Island, GA
02/2015	55 th Sanibel Symposium, St. Simons Island, GA
02/2014	54 th Sanibel Symposium, St. Simons Island, GA
02/2013	53 rd Sanibel Symposium, St. Simons Island, GA
06/2012	South Dakota EPSCoR 2012 Research Conference, Chamberlain, SD
10/2011	ND-SD 2011 joint EPSCoR Conference, Fargo, ND
06/2011	South Dakota EPSCoR 2011 Research Conference, Chamberlain, SD

AWARD

Löwdin Postdoctoral Associate Award at the 58th Sanibel Symposium, St. Simons Island, GA

PROFESSIONAL SERVICE

Organizer

“Computational Photocatalysis: Modeling Photophysics and Photochemistry at Interfaces”
Symposium, 256th ACS National Meeting & Exposition, Boston, MA (70 speakers, 15 posters,
4-day long symposium)

Peer Reviewer

*Materials Research Bulletin, Materials Science and Engineering: B, Materials Letters,
Journal of Alloys and Compounds, Nanotechnology*