Yulun Han, Ph.D.

North Dakota State University - Department of Chemistry and Biochemistry
Phone: 605-760-7891 ● yulun.han@ndsu.edu ● https://ylnhan.github.io

Research Experience and Appointments

04/2018-Present	Postdoctoral Researcher, North Dakota State University, Fargo, ND
09/2016-04/2018	Visiting Scholar, North Dakota State University, Fargo, ND Advisor: Prof. Dmitri S. Kilin Area of Research: photoinduced chemical processes, charge carrier dynamics at interfaces of nanostructures
08/2015-07/2016	Postdoctoral Researcher, University of South Dakota, Vermillion, SD Advisor: Prof. Mary T. Berry and Prof. Stanley May Area of Research: method development and applications of nanoparticles
09/2010–08/2015	Graduate Research Assistant, University of South Dakota, Vermillion, SD Advisor: Prof. Mary T. Berry Area of Research: photofragmentation of organometallic complexes, luminescence properties of lanthanides in ionic liquids

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 Ln^{3+} Complexes in the Ionic Liquid BMICl*
09/2005-07/2009	B.S. in Applied Chemistry, Donghua University, Shanghai, China

Publications

Journal articles (30 published, 14 first-authored, 6 with advisory role†)

1. **Y. Han**, D. Kilin. Photoreactions Create Superconducting Materials. *J. Appl. Spectrosc.* 2023, 90, 639–645.

2. 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.

3. 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.

4. 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.

5. 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.

6. 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.

7. T. Vazhappilly, **Y. Han**, D. S. Kilin, D. A. Micha. Electronic Relaxation of Photoexcited Open and Closed Shell Adsorbates on Semiconductors: Ag and Ag_2 on TiO_2. *J. Chem. Phys.* 2022, 156, 10, 104705.

8. **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.

9. 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.

10. **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.

11. 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.

12. M. T. Nayakasinghe, **Y. Han**, N. Sivapragasam, D. S. Kilin, N. Oncel, U. Burghaus. Adsorption of Formic Acid on $CH_3NH_3PbI_3$ Lead-Halide Organic-Inorganic Perovskites. *J. Phys. Chem. C* 2019, 123, 37, 22873-22886.

13. 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.

14. **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.

15. 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.

16. **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.

17. M. T. Nayakasinghe, **Y. Han**, N. Sivapragasam, D. S. Kilin, U. Burghaus. Unexpected High Binding Energy of CO_2 on $CH_3NH_3PbI_3$ Lead-Halide Organic-Inorganic Perovskites via Bicarbonate Formation. *Chem. Comm.* 2018, 54, 71, 9949-9952.

18. 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.

19. **Y. Han**, D. J. Vogel, T. M. Inerbaev, P. S. May, M. T. Berry, D. S. Kilin. Photoinduced Dynamics to Photoluminescence in Ln^{3+} (Ln = Ce, Pr) doped β-$NaYF_4$ Nanocrystals Computed in basis of Non-collinear Spin DFT with Spin-orbit Coupling. *Mol. Phys.* 2018, 116, 5-6, 697-707.

20. 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.

21. **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.

22. **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.

23. 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 $CH_2(NO_2)_2$ on CNT(4,0). *Mol. Phys.* 2017, 115, 5, 674-682.

24. **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.

25. **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.

26. 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.

27. **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.

28. **Y. Han**, C. Lin, Q. Meng, F. Dai, A. G. Sykes, M. T. Berry, P. S. May. $(BMI)_3LnCl_6$ Crystals as Models for the Coordination Environment of $LnCl_3$ (Ln = Sm, Eu, Dy, Er, Yb) in 1-Butyl-3-methylimidazolium Chloride Ionic-Liquid Solution. *Inorganic Chem.* 2014, 53, 11, 5494-5501.

29. **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.

30. **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", Pacifichem 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

02/2019	59th Sanibel Symposium, St. Simons Island, GA
08/2018	256th ACS National Meeting, Boston, MA
06/2018	Excited State Processes in Electronic and Bio Nanomaterials, Santa Fe, NM
02/2018	58th Sanibel Symposium, St. Simons Island, GA
10/2017	NDSU-KU Joint Symposium, Fargo, ND
02/2017	57th Sanibel Symposium, St. Simons Island, GA
08/2016	252nd ACS National Meeting, Philadelphia, PA
02/2016	56th Sanibel Symposium, St. Simons Island, GA
02/2015	55th Sanibel Symposium, St. Simons Island, GA
02/2014	54th Sanibel Symposium, St. Simons Island, GA
02/2013	53rd 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

Advising

- Dane Hogoboom (Chemistry, North Dakota State University), 1 paper published
- Brendon Disrud (Chemistry, North Dakota State University), 2 papers published
- Dakota Junkman (Chemistry, University of South Dakota), 1 paper published
- Nick Beare (Chemistry, University of South Dakota)

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*

Computer Skills

- Programming languages: Python, Matlab
- Data Structures and Algorithms: Familiarity with concepts used in machine learning research
- Frameworks: NumPy, SciPy, Pandas, Pytorch