Yuchen Wang

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Education

- **Ph.D. in Chemistry,** Kansas State University, Manhattan, KS, USA 2019 – present
  Major Professor: Prof. Christine M. Aikens; Estimate PhD defense time: Feb 2024
- **B.Sc. in Chemistry,** Anhui Normal University, Anhui, China 2015 – 2019
  Undergraduate research supervisor: Prof. Sufan Wang

Graduate Research

- Investigating the effect of field strength and silver wire length on plasmon-enhanced N_2 dissociation using nonadiabatic dynamics and real-time TDDFT method.
- Investigating the effect of doping on plasmon-enhanced N_2 dissociation on silver nanowires using nonadiabatic dynamics and real-time TDDFT method.
- Investigating the connectivity between static fields and continuous wave fields effects on plasmon-induced H_2 activation.
- Examining the interaction between diglyme and gold nanocluster using the DFT method.
- Machine learning approaches for the structure prediction of $Au_{20}(SR)_{15}$@diglyme system.
- TDDFT+aas (approximate auxiliary function) method implementation.
- sTDDFT gradient implementation.

Teaching Experience

- Mandarin instructor in International Student Center at K-State 2022 – 2023
- Graduate teaching assistant for Chemistry I and II laboratories 2019 – 2022
- Chemistry help room teaching assistant 2019 – 2021
- Mentoring undergraduate students in Prof. Aikens lab:

  Jacqueline Pinkerton (REU program), Aidan Lindsay (REU program), Brie Luccous

Publications

- Truttmann, V.; Loxha, A.; Banu, R.; Pittenauer, E.; Malola, S.; Matus, M. F.; Wang, Y.; Ploetz, E. A.; Rupprechter, G.; Bürgi, T.; Häkkinen, H.; Aikens, C.; Barrabés, N. Directing Intrinsic Chirality in Gold Nanoclusters: Preferential Formation of Stable Enantiopure Clusters in High Yield and Experimentally Unveiling the "Super" Chirality of Au_{144} *ACS Nano* 2023 *17* (20), 20376-20386
- Wang, Y. & Aikens, C. M. Connectivity between Static Field and Continuous Wave Field Effects on Excitation-Induced H_2 Activation. *J. Phys. Chem. C* 2023, 127, 31, 15375–15384
- Wang, Y. & Aikens, C. M. Effects of Field Strength and Silver Nanowire Size on Plasmon Enhanced N_2 Dissociation *J. Phys. Chem. A* 2023, 127, 27, 5609–5619
- Wang, Y., Li, A., Pinkerton, J., & Aikens, C. M. Effects of Diglyme on Au Nanocluster Formation: Mechanism, 1H NMR, and Bonding. *J. Phys. Chem. A* 2022, 126, 42, 7598–7605
- Anderson, I. D., Wang, Y., Aikens, C. M., & Ackerson, C. J. An ultrastable thiolate/diglyme ligated cluster: $Au_{20}(PET)_{15}(DG)_2$. *Nanoscale*, *14*(25), 9134-9141.

Conferences

- Oral presentation: Implementation of energy and gradient for TDDFT-approximate auxiliary function (aas) method. Wang, Yuchen and Aikens, Christine M. Nov. 15 – Nov. 18 ACS Southwest regional meeting 2023, Oklahoma City, OK
- Poster: Implementation of energy and gradient for TDDFT-approximate auxiliary function (aas) method. Wang, Yuchen and Aikens, Christine M. Kansas Physical Chemistry Symposium. Nov. 4, 2023, Lawrence, KS
- Oral presentation: Static field and continuous wave field effects on plasmon-induced H_2 activation. Wang, Yuchen and Aikens, Christine M. ACS Fall 2023, Aug 13 – Aug 17, 2023, San Francisco, CA
- Poster: Active learning applied to constructing force fields for gold thiolate-protected nanoclusters. Wang, Yuchen and Aikens, Christine M. ACS Fall 2023, Aug 13 – Aug 17, 2023, San Francisco, CA
- Lightning talk: Active learning applied to constructing force fields for gold thiolate-protected nanoclusters. Wang, Yuchen and Aikens, Christine M. 4th Artificial Intelligence for Materials Science (AIMS) workshop. July 25 - July 27, 2023, Virtual
- Poster: Implementation of energy and gradient for TDDFT-approximate auxiliary function (aas) method. Wang, Yuchen and Aikens, Christine M. TDDFT summer school and workshop, June 29 – July 8, 2023, Newark, NJ
- Poster: Interactions between diglyme and gold clusters. Wang, Yuchen and Aikens, Christine M. ACS Fall 2022, August 21 - 25, 2022. Chicago, IL

- Poster: Effect of doping on plasmon-enhanced N_2 dissociation on silver nanowires. Wang, Yuchen and Aikens, Christine M. ACS Fall 2021, August 22 - 26, 2021. Virtual
- Poster: Effects of field strength and silver nanowire length on plasmon-enhanced N_2 dissociation. Wang, Yuchen; Li, Xiaosong and Aikens, Christine M. ACS Spring 2021, April 5-30, 2021. Virtual

Selected Awards

- Scott Fateley Memorial Award at Kansas State University April 2023
- Chemistry Alumni Graduate Student Award at Kansas State university August 2022

Programs and Software

- Gaussian, GAMESS-US, ADF, VASP, Quantum ESPRESSO, GPAW
- C++, Fortran, Python, MATLAB