

Xinju Dong

Phone: (270) 421-2167 Email: spancerdong86@gmail.com

EDUCATION

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| B.S. | Western Kentucky University, Bowling Green, Kentucky | 2014 – 2018 |
| | Major: Chemistry (ACS certificate) | |
| | GPA: Cumulative 3.8; Major 3.8 | |
| M.S. | University of Louisville, Louisville, Kentucky | 2018 – 2020 |
| | Major: Chemistry | |
| | GPA: 3.8 | |
| Ph.D | University of Louisville, Louisville, Kentucky | 2021 – 2023 |
| | Major: Chemistry | |
| Postdoc | Oak Ridge National Laboratory, Oak Ridge, Tennessee | 2024 – Current |

RESEARCH WORK EXPERIENCE

Undergraduate Research Assistant: Western Kentucky University, Bowling Green, KY (Aug 2015 –May 2018)

Creation of an Interdisciplinary Platform for Renewable Solar Fuel Production (2015-2017) Advisor: Cao Yan

- Primary assistant synthesizing TiO₂ nanotube arrays with photo-responsive properties on titanium foil;
- Instrumental in evaluating, testing, and analyzing complex data for trends and statistical significance;
- Maintained and troubleshoot laboratory equipment individually, or with customer support center.

Enhancement of Solar Fuel Productivity and Energy Consumption Saving (2015-2017) Advisor: Cao Yan

- Coordinated lab responsibilities among team members to forward research agenda and solve problems;
- Synthesized improved photocatalytic nanocomposites of TiO₂ with reduced graphene oxide;
- Achieved experiment results resulting in a 20% increase of performance of photosensitive material.
- Provided clear quantitative analytical chemistry conclusions through extensive analyzing and testing.

Laboratory Support Activities:

- Aided current projects with the use of software including Gaussian in analyzing molecule's vibrations and rotation modes with different simulation methods.
- Interpreted and clarified graphs generated from UV-vis, IR, MS, LCMS, GCMS, and HPLC for team.
- Prepared samples for laboratory partners IAW complex, exacting, procedures.
- Transposed experiment raw data, into readable sketch graphs, and analyses for the team to use.

Graduate Research Assistant: University of Louisville, Louisville, KY (Aug 2018 – Dec 2023)

Global mapping of self-consistent field solution space (2018-present): Advisor: Lee M. Thompson

- Algorithms to locate solutions to self-consistent field equations for use as a basis state in post-Hartree-Fock method;
- Writing efficient code (Fortran 90/77) for characterization of the self-consistent field energy landscape.

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- Implementation of single orbital entropy and mutual information to differentiate multiple correlation mechanisms from disconnectivity graph project.

Time-dependent non-orthogonal method vs orthogonal method study (Dec 2021- Dec 2023): Advisor: Lee M.Thompson

- Data analysis in orthogonal and non-orthogonal configuration interaction methods
- Using the patterns identified to explore whether the non-orthogonal method is better than orthogonal method that can achieve accuracy with lower computational cost under real-time time-dependent context.

SKILLS

Professional:

Skilled and experienced with acquiring and interpreting analytical data, and preparing reports.

Trained in materials characterization techniques including: optical techniques, SEM, ICP (Inductively Coupled Plasma), FTIR, TGA (weight change along with time, N₂), LCMS, GC, UV-vis, and building effective photometric titration instruments on-site in lab.

Computational:

Computer programming: Mathematica, Gaussian, Origin, Fortran, Python, Perl, MATLAB, DALTON, GAMESS, Microsoft Office (Word, Excel, PowerPoint, and associated Office Suite technology).

Relational:

Mentored seamless integration of new students to university and chemistry lab;

Bilingual: English, Chinese;

Able to exhibit strong relationship, self-management, and social awareness abilities.

Teaching:

Experienced in teaching undergraduate chemistry labs; training two undergraduates' research in computational chemistry; training the first-year doctoral student

PUBLICATIONS

- Dong, X., & Thompson, L. M. Time propagation of electronic wavefunctions using nonorthogonal determinant expansions. *The Journal of Chemical Physics*, **2024**, 160(2).
- Dong, X., & Thompson, L. M. Connections Between the Self-Consistent Field Energy Landscape and Electron Correlation Mechanisms Using a Symmetry-Based Graphical Approach. **2024**, In Progress.

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- Dong, X., Mahler, A. D., Kempfer-Robertson, E. M., & Thompson, L. M. Global Elucidation of Self-Consistent Field Solution Space Using Basin Hopping. *Journal of Chemical Theory and Computation*, **2020**, *16(9)*, 5635-5644.
- Zhou, H., Ge, T., Li, H., Fang, T., Li, H., Shi, Y., ... & Dong, X. A Multi-Medium Analysis of Human Health Risk of Toxic Elements in Rice-Crayfish System: A Case Study from Middle Reach of Yangtze River, China. *Foods*, **2022**, *11(8)*, 1160.
- Min, X., Ge, T., Li, H., Shi, Y., Fang, T., Sheng, B., ... & Dong, X. Combining impregnation and co-pyrolysis to reduce the environmental risk of biochar derived from sewage sludge. *Chemosphere*, **2022**, *290*, 133371.
- Li, H., Wu, W., Min, X., Zhan, W., Fang, T., Dong, X., & Shi, Y. Immobilization and assessment of heavy metals in chicken manure compost amended with rice straw-derived biochar. *Environmental Pollutants and Bioavailability*, **2021**, *33(1)*, 1-10.
- Li, H., Yang, Z., Dai, M., Diao, X., Dai, S., Fang, T., & Dong, X. Input of Cd from agriculture phosphate fertilizer application in China during 2006–2016. *Science of the Total Environment*, **2020**, *698*, 134149.
- Li, H., Xu, W., Dai, M., Wang, Z., Dong, X., & Fang, T. Assessing heavy metal pollution in paddy soil from coal mining area, Anhui, China. *Environmental monitoring and assessment*, **2019**, *191(8)*, 1-11.
- Li, H., Min, X., Dai, M., & Dong, X. The biomass potential and GHG (Greenhouse Gas) emissions mitigation of straw-based biomass power plant: A case study in Anhui Province, China. *Processes*, **2019**, *7(9)*, 608.
- Li, H., Dai, M., Dai, S., Dong, X., & Li, F. Methylene blue adsorption properties of mechanochemistry modified coal fly ash. *Human and Ecological Risk Assessment: An International Journal*, **2018**, *24(8)*, 2133-2141.
- Dai, S., Li, H., Yang, Z., Dai, M., Dong, X., Ge, X., ... & Shi, L. Effects of biochar amendments on speciation and bioavailability of heavy metals in coal-mine-contaminated soil. *Human and Ecological Risk Assessment: An International Journal*, **2018**, *24(7)*, 1887-1900.
- Li, H., Dai, M., Dai, S., & Dong, X. Current status and environment impact of direct straw return in China's cropland—A review. *Ecotoxicology and Environmental Safety*, **2018**, *159*, 293-300.
- Chen, Y., Gao, H., Xiang, J., Dong, X., & Cao, Y. Enhanced photocatalytic activities of TiO₂-reduced graphene oxide nanocomposites controlled by Ti-O-C interfacial chemical bond. *Materials Research Bulletin*, **2018**, *99*, 29-36.
- Chen, Y., Gao, H., Wei, D., Dong, X., & Cao, Y. Langmuir-Blodgett assembly of visible light responsive TiO₂ nanotube arrays/graphene oxide heterostructure. *Applied Surface Science*, **2017**, *392*, 1036-1042.
- Chen, Y., Dong, X., Cao, Y., Xiang, J., & Gao, H. Enhanced photocatalytic activities of low-bandgap TiO₂-reduced graphene oxide nanocomposites. *Journal of Nanoparticle Research*, **2017**, *19(6)*, 1-13.

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PRESENTATIONS

- Xinju,Dong, Lee.Thompson. (2023). Understanding of Correlation Mechanisms Through Disconnectivity Graph, San Francisco, CA.
- Xinju,Dong, Lee.Thompson. (2023). Real-time Time-dependent Non-orthogonal Configuration Interaction, ACS Meeting, Indianapolis, IN.
- Xinju,Dong, Lee.Thompson. (2022). Exploring the Self-Consistent Field (SCF) Energy Landscape as a Tool for Identifying New Forms of Reference Wavefunctions, ACS Meeting, Chicago, IL.
- Xinju,Dong, Lee.Thompson. (2021). Global Searching of Self-Consistent Field Solutions Extended to Large Systems, SERMACS 2021 Regional Meeting, Birmingham, AL.
- Xinju,Dong, Lee.Thompson. (2021). Global Elucidation Approached for the Self-Consistent Field Solution Space of Molecules, ACS Oral Presentation online.
- Xinju,Dong, Lee.Thompson. (2019). Basin hopping approach to global exploration of self-consistent field solution space, SERMACS 2019 Regional Meeting, Knoxville, TN.