

Youlin Liu

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Overview: *An analytical chemistry PhD student with passion for big data analytics in chemical industry*

- Research experience in spectroscopic image analysis, chemometrics, physics modeling with relevant statistical methods
- Interdisciplinary problem solving driven combining broad chemistry knowledge and coding skills
- Documentation system management with scripting languages on an aesthetics level
- Comfortable communicating complex data to lay and technical audiences in written, verbal, and visual formats

Education

Purdue University

PhD in Chemistry (expected)

West Lafayette, Indiana

2016–present

University of Science and Technology of China (USTC)

Bachelor of Science, Chemistry

Hefei, China

2012–2016

Projects

Simpson Lab of Nonlinear Optics

Graduate Researcher

Purdue University

11/2016–present

Hyperspectral infrared imaging microscope design and digital image analysis

- Aligned optical components for a microscope to achieve co-propagation of a visible beam with an IR beam
- Managed and trouble-shoot electronics for synchronized digitization across signal acquisition
- Use different ML methods for digital image processing, classification tasks

Generative Adversarial Linear Discriminant Analysis

- Modeled a statistical probability model
- Designed coding blocks for the iterative optimization

Physics Encoded Neural Networks(PENN) for protein-matrix interactions

- Modeled an untraditional artificial neural network as a regression model with complex layer design for incorporated physics level parameters with experimental measurables
- Tested and validated DLVO model with simulated FRAP (Fluorescence recovery after photobleaching) data
- Assessed model accuracy with multivariate analysis

Synchrotron X-ray damage analysis with non-negative matrix factorization

- Performed X-ray diffraction experiments at Argonne National Laboratory
- Converted Synchrotron raw data to Matlab accessible images for in-house analysis
- Indexed peaks with XDS, HKL2000

DNA-Enabled-Nano-Group, USTC

Undergraduate Researcher

Hefei, China

05/2015–06/2016

SERS (Surface-enhanced Raman spectroscopy) with gold nanoparticles

- Optimized inorganic synthesis via reaction control
- Characterized gold dimers for plasmonic properties

Mesoscale Chemical Systems, University of Twente

Research Intern

Enschede, The Netherlands

06/2015–08/2015

Sonochemical effects analysis with microfluidic sonochemical reactor

- Designed and conducted experiments to analyze sonochemical effects with chemiluminescence
- Analyzed large amount of data for statistical significance
- Validated a microfluidic sonochemical reactor's capability for producing localized radicals

Environmental Engineering Laboratory, USTC

Undergraduate Researcher

Hefei, China

01/2014–04/2015

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SeCd Quantum dots detoxification analysis in C. elegans

- Toxicity analysis with SeCd forming to quantum dots within C. elegans
- Characterization methods: HPLC, fluorescence microscopy

Skills & Interests

Laboratorial: Standard inorganic&organic synthesis, optical path alignment, X-ray diffraction operation

Proficient coding languages: Matlab, python

Typesetting and documentation management: L^AT_EX, Markdown, html, pandoc, git, bash

Other standalone suites: LabView, XDS, HKL2000, CCP4, Vina, ImageJ

Outreach & Teaching

Singer: Performed acoustic guitar song covers at local open mic nights	2019-present
Dancer: Member of D.A.O. (Purdue Dance All Out Club) and performed at invited events	2018-present
Teaching Assistant: General chemistry teaching assistant, Purdue University	2017-2018
Course Coordinator: General chemistry II course coordinator for interactive teaching	2018
Graduate TA Mentor: Guidance and feedback to new graduate teaching assistants	2018-2019
Volunteer: National Chemistry Week	2016-2019
Hostess: Hostess for Stanford-USTC-MIT evening open dialogue with USTC students	2013

Conferences

Scix Generative Adversarial Linear Discriminant Analysis	(virtual) 2020
ACS Generative Adversarial Linear Discriminant Analysis	San Diego, CA (virtual) 2020
Pittcon Conference Hyperspectral image classification	Chicago, IL 2020
Turkey Run Analytical Chemistry Conference Adversarial Spectroscopy	Marshall, IN 2019
Pittcon Conference Hyperspectral IR imaging	Philadelphia, PA 2019

Publications

Liu, Y., Smith, C., Cao, Z., Sherman, A., & Simpson, G. J. "Generative Adversarial Linear Discriminant Analysis" (in revision)

"High-throughput fluorescence recovery after photobleaching diffusion analysis of protein/excipient interactions" (manuscript in preparation)

Sarkar, S., Florian, H., Liu, Y., Geiger, A. & Simpson, G. J. "Non-negative Matrix Factorization for Isolating Damage-Free Reflections in Macromolecular Synchrotron Data Collection" (manuscript in preparation)

Smith, C., Liu, Y., & Simpson, G. J. "Defense against adversarial spectroscopic attacks" (Conference Presentation). In Big Data: Learning, Analytics, and Applications (Vol. 10989, p. 109890F). International Society for Optics and Photonics.

Geiger, A. C., Ulcickas, J. R., Liu, Y., Witinski, M. F., Blanchard, R., & Simpson, G. J. "Sparse-sampling methods for hyperspectral infrared microscopy". In Image Sensing Technologies: Materials, Devices, Systems, and Applications VI (Vol. 10980, p. 1098016). International Society for Optics and Photonics.

Verhaagen, Bram, Youlin Liu, Andrés Galdames Pérez, Elena Castro-Hernandez, & David Fernandez Rivas. "Scaled-up sonochemical microreactor with increased efficiency and reproducibility." ChemistrySelect 1, no. 2 (2016): 136-139.