# Youlin Liu

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

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

#### **Education**

**Purdue University** 

West Lafayette, Indiana

PhD in Chemistry (expected)

2016-present

**University of Science and Technology of China (USTC)** 

Hefei, China

Bachelor of Science, Chemistry

2012-2016

## **Projects**

## **Simpson Lab of Nonlinear Optics**

**Purdue University** 

Graduate Researcher

11/2016-present

## Hyperspectral infrared imaging microscope design and digital image analysis

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

### Generative Adversarial Linear Discriminant Analysis

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

### Physics Encoded Neural Networks(PENN)

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

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

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

### DNA-Enabled-Nano-Group, USTC

Hefei, China

Undergraduate Researcher

05/2015-06/2016

### SERS (Surface-enhanced Raman spectroscopy) with gold nanoparticles

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

# Mesoscale Chemical Systems, University of Twente

**Enschede, The Netherlands** 

Research Intern

06/2015-08/2015

### Sonochemical effects analysis with microfluidic sonochemical reactor

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

## **Environmental Engineering Laboratory, USTC**

Hefei, China

*Undergraduate Researcher* 

01/2014-04/2015

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## SeCd Quantum dots detoxification analysis in C. elegans

- o Toxicity analysis with SeCd forming to quantum dots within C. elegans
- o 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: LATEX, Markdown, html, pandoc, git, bash

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

## **Awards**

o Outstanding USTC student awards, $2^{nd}$ metalist in 2013, $3^{rd}$ in 2014&2015	
o CSC (China Scholarship Council) Full Scholarship for summer intern in Europe	2015

## **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
<b>Volunteer:</b> International communication voluntary group in USTC	2013-2016

#### **Conferences**

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" (submitted)

Smith, C., Liu, Y., & Simpson, G. J. (2019, May). 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. (2019, May). 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, and David Fernandez Rivas. "Scaled—up sonochemical microreactor with increased efficiency and reproducibility." ChemistrySelect 1, no. 2 (2016): 136-139.