

# Youlin Liu

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

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- Research experience in spectroscopic image analysis, physics modeling with machine learning 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

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### 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

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### 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 electronics for synchronized digitization of the microscope
- Used both traditional and machine learning classification methods and successfully classified clopidogrel form 1 and form 2 as an testing example

#### *Adversarial spectroscopy*

- Optimized a genetic algorithm for iteration
- Modeled a traditional statistical probability calculation function as a testing metric
- Optimized a LDA (Linear Discriminate Analysis) algorithm in consideration of the SSS (small sample size) problem

#### *Molecular level protein interaction modeling with experimental observables*

- 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 the model with simulated FRAP (Fluorescence recovery after photobleaching) data

#### *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 the 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
- Used DLS (Dynamic Light Scattering), UV-Vis, gel electrophoresis for characterization of the gold dimers

### 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 the 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
- Maintenance of C. elegans in the laboratory

## Skills & Interests

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

**Familiar python packages:** Keras, Scikit, Tensorflow

**Proficient coding languages:** Matlab, python

**Typesetting and documentation management:** L<sup>A</sup>T<sub>E</sub>X, Markdown, html, pandoc, git, bash

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

## Awards

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- Outstanding USTC student awards, 2<sup>nd</sup> metalist in 2013, 3<sup>rd</sup> in 2014&2015
- CSC (China Scholarship Council) Full Scholarship for summer intern in Europe 2015

## Outreach & Teaching

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**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

**Volunteer:** International communication voluntary group in USTC 2013-2016

## Honors Societies

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**Phi Lambda Upsilon** National Honorary Chemistry Society 2016-present

**Iota Sigma Pi** National Honor Society for Women in Chemistry 2016-present

## Conferences

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**Pittcon** Hyperspectral image classification 2020

**Turkey Run** Adversarial Spectroscopy 2019

**Pittcon** Hyperspectral IR imaging 2019

## Publications

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Smith, Casey and **Liu, Youlin** and Simpson, Garth J, *Adversarial Spectroscopy (in review)*

Sarkar, Sreya; Florian, Hilary; **Liu, Youlin**; Geiger, Andreas; Simpson, Garth; *Non-Negative Matrix Factorization for Isolating Damage-Free Reflections in Macromolecular Synchrotron Data Collection (in review)*

Smith, Casey and **Liu, Youlin** and Simpson, Garth J, Big Data: Learning, Analytics, and Applications, 2019, 10989, 109890F

Bram Verhaagen, **Youlin Liu**, Andrés Galdames Pérez, Elena Castro-Hernandez, David Fernandez Rivas, ChemistrySelect 2016, 1, 136.