Youlin Liu

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

- 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

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

- 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 relation to 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 — Hefei, China
Undergraduate Researcher — 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 — Enschede, The Netherlands
Research Intern — 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

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Environmental Engineering Laboratory, USTC — Hefei, China
Undergraduate Researcher — 01/2014–04/2015
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

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

Familiar python packages: Pandas, OpenCV, Keras, Scikit, Tensorflow

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

- Outstanding USTC student awards, 2^{nd} metalist in 2013, 3^{rd} in 2014&2015
- 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
Volunteer: International communication voluntary group in USTC	2013-2016

Conferences

Pittcon Hyperspectral image classification	2020
Turkey Run Adversarial Spectroscopy	2019
Pittcon Hyperspectral IR imaging	2019

Publications

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.