YUE YU

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EDUCATION

University of Kentucky, Lexington, KY *May. 2018*
Ph.D in Chemical Engineering Overall GPA: 4.0/4.0
Thesis title: *Understanding inhibition mechanism for biological desulfurization to improve sulfur removal from petroleum oil*
Advisor: Prof. Christina M. Payne

University of Kentucky, Lexington, KY *May. 2014*
B.S. in Chemical Engineering Overall GPA: 3.7/4.0
With university honors

China University of Mining and Technology, Xuzhou, China *May. 2014*
B.S. in Process Equipment and Control Engineering Overall GPA: 3.6/4.0

EMPLOYMENT AND EXPERIENCE

University of California, Merced, CA *Nov. 2021 — Present*
Sr. Research Computing Facilitator *Supervisor: Sarvani Chadalapaka*

· Conduct complex research computing systems design and management
· Teach and train high performance computing topics (service including entire central valley of California) to enable broad research computing engagement

University of California, Merced, CA *Jan. 2019 — Oct.2021*
Postdoctoral Scholar *Advisor: Prof. Liang Shi*

· Designed multi-scale molecular modeling schemes for complex system
· Developed complex computing algorithms for spectral modeling of photovoltaic materials to enhance the broader application of renewable energy

Virginia Tech, Blacksburg, VA *Jan. 2018 — Jan. 2019*
Postdoctoral Associate *Advisor: Prof. Justin A. Lemkul*

· Designed GPU-accelerated calculation protocol
· Constructed automated computer tool to identify protein structure aim to identify Alzheimer disease at early stage

Swedish Univ. of Agricultural Science (SLU), Uppsala, Sweden *Jun. 2016 — Aug. 2016*
Invited Guest Researcher *Advisor: Prof. Mats Sandgren*

· Applied various computer techniques to predict small molecules binding position inside protein
· Engaged in computation and experiment collaborations for complex systems structure prediction

University of Kentucky, Lexington, KY *Aug. 2014 — Dec. 2017*
Graduate Research Assistant *Advisor: Prof. Christina M. Payne*

· Developed force field parameterization schemes for drug-like molecules
· Determined mechanisms to enhance petroleum biodesulfurization process

AWARDS

Apr. 2021	XSEDE (eXtreme Science and Engineering Discovery Environment) Provision Award with 13,200.0 GPU Hours and 144,000.0 Core-hours, the estimated value is $9500
Jan. 2020	XSEDE start-up grant, 50000 Core-hours and 2500 GPU hours with 500 GB storage, the estimated value is $2000
Nov. 2016	1st Place poster award among over 100 attendees in Distinguished Lectures and Drug Discovery and Development Symposium by *Ashland Inc.*

PROFESSIONAL MEMBERSHIPS

Dec. 2021 - Present	Certified instructor for Carpentries workshops
Nov. 2021 - Present	XSEDE Campus Champion
July 2022 - Present	XSEDE Resource Allocation Committee (XRAC)
June 2019 - June 2021	American Chemical Society (ACS)
May 2014 - Aug. 2017	American Institute of Chemical Engineers (AIChE)

TEACHING AND MENTORING EXPERIENCE

PEARC22 Student Program (SP) *July 2022 — July 2022*
Mentor *PEARC22, Boston*

· Supervised selected university student nationwide to help the student with the professional development
· Conducted discussions with other mentors for service enhancement of SP program

ACS SEED Program *Jun. 2019 — Aug. 2019*
Mentor *University of California, Merced*

· Supervised high school students with little computational background, by the end of the program the student had achieved advanced research task independently
· Designed the entire training workflow for high school students

CME 462 - Process Control *Jan. 2015 — May. 2015*
Teaching Assistant - junior level class with 40 students *University of Kentucky*

· Served as primary instructor for several lectures
· Graded homework and exams, and led the discussion sessions
· Received very positive feedback from students and the primary instructor

CME 433 - Chemical Engineering Lab *Aug. 2014 — Dec. 2014*
Teaching/Lab Assistant - senior level class with 30 students *University of Kentucky*

· Contributed to mentoring senior chemical engineering undergraduates for final graduating projects
· Graded and critiqued lab reports
· Designed and instructed labs

Microteaching Training Leader *Aug. 2015 — Aug. 2015*
TA Training Leader - group study leader for 8 Ph.D candidates *University of Kentucky*

· Trained newly enrolled university-wide graduate students teaching techqiues
· Led the teaching sessions for new Ph.D candidates
· Provided critiques for final te404711034aching projects

PEER-REVIEWED PUBLICATIONS

- Yue Yu, and Liang Shi, "Molecular disorder at the PCBM/P3HT interface revealed by infrared spectroscopy of ester carbonyl stretch" (to be submitted)
- Biyue Zhu, Jing Yang, Richard Van, Fan Yang, Yue Yu, Astra Yu, Kathleen Ran, Keyi Yin, Yingxi Liang, Xunuo Shen, Wei Yin, Se Hoon Choi, Ying Lu, Changning Wang, Yihan Shao, Liang Shi, Rudolph E. Tanzi, Can Zhang, Yan Cheng, Zhirong Zhang, and Chongzhao Ran, "Epitope alteration by small molecules and applications in drug discovery", *Chemical Science*, **13**, 8104 (2022)
- Chao Zheng, Yue Yu, Shi Kuang, Biyue Zhu, Heng Zhou, Shao-Qing Zhang, Jing Yang, Liang Shi, and Chonzhao Ran, "β-Amyloid peptides manipulate switching behaviors of donor–acceptor stenhouse adducts", *Analytical Chemistry*, **93**, 9887 (2021)
- Chee-Kong Lee, Chengqiang Lu, Yue Yu, Qiming Sun, Chang-Yu Hsieh, Shengyu Zhang, Qi Liu, and Liang Shi, "Transfer learning with graph neural networks for optoelectronic properties of conjugated oligomers", *The Journal of Chemical Physics*, **154**, 024906 (2021)
- Yue Yu, and Liang Shi, "Vibrational solvatochromism of the ester carbonyl vibration of PCBM in organic solutions", *The Journal of Chemical Physics*, **151**, 064501 (2019)
- Yue Yu, Landon C. Mills, and Christina M. Payne, "Inhibition mechanisms of rhodococcus erythropolis 2'-hydroxybiphenyl 2-sulfinate desulfinase (DszB)", *Journal of Physical Chemistry B*, **123**, 9054 (2019)
- Yue Yu, Ishan Fursule, Landon C. Mills, Derek L. Englert, Brad J. Berron, and Christina M. Payne, "CHARMM force field parameters for 2'-hydroxybiphenyl-2-sulfinate, 2- hydroxybiphenyl, and related analogs", *Journal of Molecular Graphics and Modelling*, **72**, 32 (2017)

PRESENTATIONS

- Yue Yu, and Liang Shi, *"Unveiling the molecular structure of the P3HT/PCBM interface by infrared spectroscopy of ester carbonyl stretch"* Virtual Spring 2021 ACS National Meeting & Exposition, Apr. 2021
- Yue Yu, and Liang Shi, *"Molecular disorder at donor/acceptor interface of P3HT/PCBM"*, Virtual Conference on Theoretical Chemistry 2020 (VCTC), July 2020
- Yue Yu, and Liang Shi, *"Modeling vibrational spectroscopy of orgainic photovoltaic materials"*, Fall ACS National Meeting & Exposition, San Diego, CA, Aug. 2019
- Yue Yu, and Justin A. Lemkul, *"Helix-coil equilibrium in alanine-based model peptides: implications for protein folding"*, Computer-aided drug design symposium, Baltimore, MD, May. 2018
- Yue Yu, and Christina M. Payne, *"Conformational changes of 2'-hydroxybiphenyl-2-sulfinate desulfinase"*, 2017 AIChE Annual Meeting, Minneapolis, MN, Oct. 2017
- Yue Yu, and Christina M. Payne, *"Molecular dynamics simulations revealed conformational change in 2'-hydroxybiphenyl-2-sulfinate (HBPS) desulfinase"* Ashland Inc. Distinguished Lectures and Drug Discovery and Development Symposium, Lexington, KY, Nov. 2016 (**the first prize poster**)
- Yue Yu, and Christina M. Payne, *"The relations between conformational changes in 2'-hydroxybiphenyl sulfinate desulfinase to product inhibition"*, Midwest Enzyme Chemistry Conference, Chicago, IL, Oct. 2016
- Yue Yu, and Christina M. Payne, *"Force field parameterization of 2'-hydroxybiphenyl-2-sulfinate, 2-hydroxybiphenyl, and related analogs"*, 20$^{\text{th}}$ Swedish Conference on Protein Structure and Function (SBNet), Tällberg, Sweden, Jun. 2016
- Yue Yu, Ishan Fursule, Landon C. Mills, Derek L. Englert, Bradley J. Berron, and Christina M. Payne, *"CHARMM additive all-atom force field for 2-(2'-hydroxyphenyl) benzenesulfinate, 2-hydroxybiphenyl and related analogs"*, 2016 Materials and Chemical Engineering Graduate Students Spring Syposium, Lexington, KY, May 2016

TECHNICAL SKILLS

Computer Languages	Python, C, C++, R, Bash, FORTRAN, Perl, MATLAB
Software & Tools	GROMACS, CHARMM, NAMD, OpenMM, Amber, VMD, Pymol, Gaussian, HTML, LaTeX, MS Offics Suite, Mathematica, ASPEN Plus

REFERENCES

1. Dr. Liang Shi, Assistant Professor
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   lshi4@ucmerced.edu
2. Dr. Justin A. Lemkul, Assistant Professor
   Virginia Tech
   340 West Campus Dr., Blacksburg, VA
   jalemkul@vt.edu
3. Dr. Christina M. Payne, Program Director
   National Science Foundation
   2415 Elsenhower Ave., Alexandria, VA
   cpayne@nsf.gov