

Curriculum Vitae

Kevin (Shih-Hsien) Liu (劉士賢)

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Objective A research professional with chemical engineering background and experience in physical and computational chemistry for biological applications.
Research interests: drug discovery, bioenergy, nanoscience, and molecular dynamics.

Work **3. Postdoctoral Research Associate, Oak Ridge National Laboratory** Aug. 2017-Present
Center for Molecular Biophysics

- Drug discovery: designing small-molecule inhibitors of protein-protein (FGF23- α -Klotho) interactions to treat kidney disease and inhibitors of RNA-dependent RNA polymerase in SARS-CoV-2 to treat COVID-19 using molecular dynamics (MD) simulations, flexible ligand docking and virtual screening, and collaborating with medicinal chemists and virologists at the University of Tennessee Health Science Center
- Bioenergy: resolving structure-property relationships of lignocellulosic polymers for biomass utilization using MD simulations and machine learning, and collaborating with experimentalists in Manufacturing and Neutron Sciences at ORNL
- Agrochemical: resolving structure-property relationships of zinc-based nano-therapeutics for citrus greening disease using MD simulations, and collaborating with experimentalists at NanoScience Technology Center, University of Central Florida

2. Graduate Research Assistant, The Pennsylvania State University Aug. 2011-Aug. 2017
Department of Chemical Engineering

- Developed pair and many-body interatomic potentials for the adsorption of primary alkylamines on Cu surfaces with Python-coded simulated annealing for MD simulations
- Resolved structure-property relationships at metal-organic (Au-PVP and Cu-HDA) interface with DFT/MD on Linux high performance computing (HPC) clusters
- Proved experimental hypothesis of shape-selective syntheses of Au and Cu nanocrystals with DFT/MD for applications in catalysis and flexible transparent conducting films

1. Graduate Research Assistant, National Taiwan University Jul. 2007-Jul. 2010
Department of Chemical Engineering

- Fabricated and characterized CIGS and DSSC photovoltaic (PV) devices
 - Prepared CuInSe₂ thin films by selenizing Cu-In alloy nanoparticles via chemical vapor deposition (CVD) process
 - Synthesized ZnO nanospheres and TiO₂ nanotubes via hydrothermal method
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Education **2. The Pennsylvania State University, University Park, PA**
Ph.D. in Computational Chemistry (*GPA: 4.00*) Aug. 2011-Aug. 2017

Dissertation: *Shape-Selective Syntheses of Gold and Copper Nanostructures: Insights from Density-Functional Theory and Molecular Dynamics*
Advisor: Kristen Fichthorn

1. National Taiwan University, Taipei, Taiwan
M.S. in Materials Chemistry (*GPA: 4.00*) Jul. 2008-Jul. 2010

Thesis: *Preparation and Characterization of Copper Indium Diselenide Thin Films*
Advisor: Chung-Hsin Lu

B.S.E. in Chemical Engineering (*GPA: 3.91*) Sep. 2004-Jun. 2008

Grant **1. "Enhancing Drug Discovery via Prediction of Hot Spots"** Oct. 2019-Sep. 2020
Principal Investigator: Loukas Petridis
Laboratory Directed Research and Development: the Seed Money Fund, \$190,000, LOIS 9910

Patent

1. "Method of Forming IB-III-A-VIA Compounds" Jul. 2012
Lu, C.-H.; **Liu, S.-H.**; Chen, F.-S.
Taiwan 201228930
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Publications

Citations: 284

h-index: 9

i10-index: 9

17. "Cellulose Nanofibrils in Spray Drying Process: Insights from Molecular-Dynamics Simulations and Small-Angle Neutron Scattering"
Liu, S.-H.; Li, K.; Lamm, M. E.; Smith, M. D.; Pingali, S. V.; Ozcan, S.; Smith, J. C.; Petridis, L.*
Cellulose (Manuscript in Preparation)
16. "Identification of Small-Molecule Inhibitors of Fibroblast Growth Factor 23 Signaling via *In Silico* Hot Spot Prediction and Molecular Docking to α -Klotho"
Liu, S.-H.[#]; Xiao, Z.[#]; Mishra, S. K.; Mitchell, J. C.; Smith, J. C.; Quarles, L. D.; Petridis, L.* ([#]equal contribution)
Journal of Chemical Information and Modeling **2022**, 62 (15), 3627-3637
15. "Novel Small Molecule Fibroblast Growth Factor 23 Inhibitors Increase Serum Phosphate and Improve Skeletal Abnormalities in *Hyp* Mice"
Xiao, Z.*; Liu, J.; **Liu, S.-H.**; Petridis, L.; Cai, C.; Cao, L.; Wang, G.; Chin, A. L.; Cleveland, J. W.; Ikedionwu, M. O.; Carrick, J. D.; Smith, J. C.; Quarles, L. D.*
Molecular Pharmacology **2022**, 101 (6), 408-421
14. "Innovative High-Feed Rate Additive Manufacturing Using Sustainable Nano/Microcellulose-Reinforced Thermoplastic Composites: Phase II 2021 Q4"
Anderson, J.; Armstrong, K.; Chowdhury, D.; Copenhaver, K.; Gramlich, W.; Johnson, D.; Lamm, M.; **Liu, S.-H.**; MacKay, S.; Ozcan, S.*; Petridis, L.; Post, B.; Roschli, A.; Sethuraman, V.; Tajvidi, M.; Tekinalp, H.; Vaidya, U.; Villez, K.; Walker, C.; Wang, L.; Wasti, S.
Oak Ridge National Laboratory Report **2021**, ORNL/SPR-2021/2343
13. "Innovative High-Feed Rate Additive Manufacturing Using Sustainable Nano/Microcellulose-Reinforced Thermoplastic Composites: Phase II 2021 Q3"
Anderson, J.; Chowdhury, D.; Copenhaver, K.; Han, Y.; Johnson, D.; **Liu, S.-H.**; MacKay, S.; Ozcan, S.*; Petridis, L.; Sethuraman, V.; Shams Es-haghi, S.; Smith, T.; Tekinalp, H.; Vaidya, U.; Villez, K.; Walker, C.; Wang, L.; Wasti, S.; Zhao, X.
Oak Ridge National Laboratory Report **2021**, ORNL/SPR-2021/2148
12. "Innovative High-Feed Rate Additive Manufacturing Using Sustainable Nano/Microcellulose-Reinforced Thermoplastic Composites: Phase II 2021 Q2"
Anderson, J.; Chowdhury, D.; Copenhaver, K.; Han, Y.; Johnson, D.; Kim, P.; Lamm, M.; **Liu, S.-H.**; MacKay, S.; Ozcan, S.*; Petridis, L.; Sethuraman, V.; Tekinalp, H.; Vaidya, U.; Villez, K.; Walker, C.; Wang, L.; Wasti, S.
Oak Ridge National Laboratory Report **2021**, ORNL/SPR-2021/2147
11. "Innovative High-Feed Rate Additive Manufacturing Using Sustainable Nano/Microcellulose-Reinforced Thermoplastic Composites: Phase II 2021 Q1"
Anderson, J.; Copenhaver, K.; Han, Y.; Johnson, D.; Kerr, J.; Kim, P.; Lamm, M.; Li, K.; **Liu, S.-H.**; MacKay, S.; Ozcan, S.*; Petridis, L.; Post, B.; Sethuraman, V.; Tekinalp, H.; Vaidya, U.; Villez, K.; Wang, L.
Oak Ridge National Laboratory Report **2021**, ORNL/SPR-2021/1835
10. "Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19"
Acharya, A.; Agarwal, R.; Baker, M. B.; Baudry, J.; Bhowmik, D.; Boehm, S.; Byler, K. G.; Chen, S. Y.-C.; Coates, L.; Cooper, C. J.; Demerdash, O.; Daidone, I.; Eblen, J. D.; Ellingson, S.; Forli, S.; Glaser, J.; Gumbart, J. C.; Gunnels, J.; Hernandez, O.; Irle, S.; Kneller, D. W.; Kovalevsky, A.; Larkin, J.; Lawrence, T. J.; LeGrand, S.; **Liu, S.-H.**; Mitchell, J. C.; Park, G.; Parks, J. M.; Pavlova, A.; Petridis, L.; Poole, D.; Pouchard, L.; Ramanathan, A.; Rogers, D. M.; Santos-Martins, D.; Scheinberg, A.; Sedova, A.; Shen,

Y.; Smith, J. C.*; Smith, M. D.; Soto, C.; Tsaris, A.; Thavappiragasam, M.; Tillack, A. F.; Vermaas, J. V.; Vuong, V. Q.; Yin, J.; Yoo, S.; Zahran, M.; Zanetti-Polzi, L. *Journal of Chemical Information and Modeling* **2020**, *60* (12), 5832-5852

9. "Deconstruction of Biomass Enabled by Local Demixing of Cosolvents at Cellulose and Lignin Surfaces"
Pingali, S. V.; Smith, M. D.[#]; **Liu, S.-H.**[#]; Rawal, T. B.[#]; Pu, Y.; Shah, R.; Evans, B. R.; Urban, V. S.; Davison, B. H.; Cai, C. M.; Ragauskas, A. J.; O'Neill, H. M.; Smith, J. C.; Petridis, L.* ([#]equal contribution)
Proceedings of the National Academy of Sciences **2020**, *117* (29), 16776-16781
8. "Ammonia-Salt Solvent Promotes Cellulosic Biomass Deconstruction Under Ambient Pretreatment Conditions to Enable Rapid Soluble Sugar Production at Ultra-Low Enzyme Loadings"
Chundawat, S. P. S.*; da Costa Sousa, L.; Roy, S.; Yang, Z.; Gupta, S.; Pal, R.; Zhao, C.; **Liu, S.-H.**; Petridis, L.; O'Neill, H.; Pingali, S. V.
Green Chemistry **2020**, *22* (1), 204-218
7. "Interaction of Zinc Oxide Nanoparticles with Water: Implications for Catalytic Activity"
Rawal, T. B.; Ozcan, A.; **Liu, S.-H.**; Pingali, S. V.; Akbilgic, O.; Tetard, L.; O'Neill, H.; Santra, S.; Petridis, L.*
ACS Applied Nano Materials **2019**, *2* (7), 4257-4266
6. "Antimicrobial Zn-Based "TSOL" for Citrus Greening Management: Insights from Spectroscopy and Molecular Simulation"
Liu, S.-H.; Rawal, T. B.; Soliman, M.; Lee, B.; Maxwell, T.; Rajasekaran, P.; Mendis, H. C.; Labbé, N.; Santra, S.; Tetard, L.; Petridis, L.*
Journal of Agricultural and Food Chemistry **2019**, *67* (25), 6970-6977
5. "Interaction of Alkylamines with Cu Surfaces: A Metal-Organic Many-Body Force Field"
Liu, S.-H.; Fichthorn, K. A.*
The Journal of Physical Chemistry C **2017**, *121* (40), 22531-22541
4. "Self-Assembled Monolayer Structures of Hexadecylamine on Cu Surfaces: Density-Functional Theory"
Liu, S.-H.; Balankura, T.; Fichthorn, K. A.*
Physical Chemistry Chemical Physics **2016**, *18* (48), 32753-32761
3. "Synthesis of {111}-Faceted Au Nanocrystals Mediated by Polyvinylpyrrolidone: Insights from Density-Functional Theory and Molecular Dynamics"
Liu, S.-H.; Saidi, W. A.; Zhou, Y.; Fichthorn, K. A.*
The Journal of Physical Chemistry C **2015**, *119* (21), 11982-11990
2. "Synthesis of CuInSe₂ Films via Selenizing the Cu-In Alloy-Containing Nanopowders"
Liu, S.-H.; Chen, F.-S.; Lu, C.-H.*
Journal of Alloys and Compounds **2012**, *517*, 14-19
1. "Preparation of Thin CuInSe₂ Films Using Cu-In Alloy Nanoparticles"
Liu, S.-H.; Chen, F.-S.; Lu, C.-H.*
Chemistry Letters **2010**, *39* (12), 1333-1335

Presentations

4. "Antimicrobial Properties and Molecular Structures of TSOL"
Liu, S.-H. *et al.* *Materials Innovation for Sustainable Agriculture Symposium* **2018**
 3. "PVP Facilitates {111}-Faceted Au Nanocrystals Formation: Insights from DFT and MD"
Liu, S.-H. *et al.* *TechConnect World Innovation Conference* **2015**
 2. "Shape-Selective Synthesis of Au Nanoparticles: The Role of PVP"
Liu, S.-H. *et al.* *AIChE Annual Meeting* **2013**
 1. "DFT Calculations of the Role of PVP in the Controlled Synthesis of Au Nanostructures"
Liu, S.-H. *et al.* *APS March Meeting* **2013**
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Teaching Experience	<p>Graduate Teaching Assistant, <i>The Pennsylvania State University</i> Department of Chemical Engineering</p> <p>5. CH E 470, Process Design of Chemical Plants Jan. 2017-May 2017</p> <p>4. CH E 524, Molecular Thermodynamics and Statistical Mechanics Aug. 2016-Dec. 2016</p> <p>3. CH E 480, Chemical Engineering Laboratory Aug. 2015-May 2016</p> <ul style="list-style-type: none"> • Demonstrated the unit operations experiments to ~100 undergraduate students • Taught background theory and data processing on the experiments for ~8 hours a week • Troubleshoot the equipment and resolved the issues with instructors and fellow TAs <p>2. CH E 210, Introduction to Material Balances Jan. 2015-May 2015</p> <p>1. CH E 320, Phase and Chemical Equilibria Aug. 2013-Dec. 2013</p>
Reviewer Experience	<p>2. Book: “Extending and Modifying LAMMPS: Writing Your Own Source Code” Mubin, S.; Li, J. <i>Packt Publishing Ltd.</i> 2021 Oct. 2020-Jan. 2021</p> <p>1. Journal article: “Two-Dimensional Wetting Transition Modeling with the Potts Model” Lopes, D. M.; Mombach, J. C. M. <i>Brazilian Journal of Physics</i> 2017, 47, 672-677 Jul. 2017-Oct. 2017</p>
Skills	<ul style="list-style-type: none"> • Computation: Python, Linux, Bash, GROMACS, VMD, CHARMM, AutoDock VinaMPI, PDB, MODELLER, PyMOL, MOE, Gaussian, VASP, LAMMPS, Simulated Annealing, Machine Learning • Synthesis: CVD, Chemical Reduction, Hydrothermal • Characterization: XRD, SEM, UV-Vis-NIR, Raman, ICP-MS, Solar Simulator
Languages	<ul style="list-style-type: none"> • American English, Mandarin Chinese, Taiwanese
Honors and Awards	<p>4. Oak Ridge Leadership Computing Facility Director's Discretion Project (BIP197) Dec. 2019 “Molecular Modeling of Cellulose Nanofibers in Spray Drying Process” <i>Oak Ridge Leadership Computing Facility</i></p> <p>3. Distinguished Conscript, <i>Taiwan Air Force</i> Aug. 2010-Jul. 2011</p> <p>2. Presidential Award (Honors), <i>National Taiwan University</i> Oct. 2008</p> <p>1. Undergraduate Research Project (96-2815-C-002-020-E) Jul. 2007-Feb. 2008 “Preparation and Characterization of TiO₂ Nanomaterials” <i>Taiwan National Science Council</i></p>
References	<p>Loukas Petridis petridisl@ornl.gov Staff Scientist at Center for Molecular Biophysics <i>Oak Ridge National Laboratory</i></p> <p>Jeremy Smith smithjc@ornl.gov Governor’s Chair, Director of Center for Molecular Biophysics, Professor of Biochemistry & Cellular and Molecular Biology <i>The University of Tennessee, Knoxville</i></p> <p>Swadeshmukul Santra ssantra@ucf.edu Professor of NanoScience Technology Center, Chemistry, Materials Science and Engineering, and Biomedical Sciences, Director of Materials Innovation for Sustainable Agriculture <i>University of Central Florida</i></p> <p>Darryl Quarles dquarles@uthsc.edu UTMG Endowed Professor, Director of Division of Nephrology in Department of Medicine, Associate Dean for Research in College of Medicine</p>

The University of Tennessee Health Science Center

Kristen Fichthorn

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Merrell Fenske Professor of Chemical Engineering and Professor of Physics

The Pennsylvania State University

Personal

Married, one child
