Kevin (Shih-Hsien) Liu

Contact Info.

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Work

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 SARS-CoV-2 (coronavirus) to treat COVID-19 using 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 molecular dynamics (MD) simulations, 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

Education

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

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

- "Enhancing Drug Discovery via Prediction of Hot Spots"
  Laboratory Directed Research and Development: the Seed Money Fund Oct. 2019
  Principal Investigator: Loukas Petridis

Patent

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

Publications

- "Identification of Small-Molecule Inhibitors of FGF23 Signaling via *In Silico* Hot Spot Prediction and Molecular Docking to α-Klotho"
  Liu, S.-H.; Xiao, Z.; Mishra, S. K. *et al.*
  ChemRxiv Preprint **2020**, DOI: 10.26434/chemrxiv.13083224
  Journal of Medicinal Chemistry (In Review)
- "Small Molecule FGF23 Inhibitors Increase Serum Phosphate and Improve Skeletal Abnormalities in *Hyp* Mice"
  Xiao, Z.; Liu, J.; **Liu, S.-H.** *et al.*
  bioRxiv Preprint **2020**, DOI: 10.1101/2020.08.04.236877
- "Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19"
  Acharya, A.; Agarwal, R.; Baker, M.;……**Liu, S.-H.** *et al.*
  ChemRxiv Preprint **2020**, DOI: 10.26434/chemrxiv.12725465
  Journal of Chemical Information and Modeling (In Revision)
- "Deconstruction of Biomass Enabled by Local Demixing of Cosolvents at Cellulose and Lignin Surfaces"
  Pingali, S. V.; Smith, M. D.; **Liu, S.-H.** *et al.*

Proceedings of the National Academy of Sciences **2020**, *117 (29)*, 16776-16781

- "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.; Costa Sousa, L.; Roy, S.;……**Liu, S.-H.** *et al.*
  Green Chemistry **2020**, *22 (1)*, 204-218
- "Interaction of Zinc Oxide Nanoparticles with Water: Implications for Catalytic Activity"
  Rawal, T. B.; Ozcan, A.; **Liu, S.-H.** *et al.*
  ACS Applied Nano Materials **2019**, *2 (7)*, 4257-4266
- "Antimicrobial Zn-Based "TSOL" for Citrus Greening Management: Insights from Spectroscopy and Molecular Simulation"
  Liu, S.-H.; Rawal, T. B.; Soliman, M. *et al.*
  Journal of Agricultural and Food Chemistry **2019**, *67 (25)*, 6970-6977
- "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
- "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
- "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
- "Synthesis of $CuInSe_2$ 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
- "Preparation of Thin $CuInSe_2$ Films Using Cu-In Alloy Nanoparticles"
  Liu, S.-H.; Chen, F.-S.; Lu, C.-H.
  Chemistry Letters **2010**, *39 (12)*, 1333-1335

Objective

- A research professional with chemical engineering background and experience in physical and computational chemistry for biological applications

Research Experience

Research Assistant, *The Pennsylvania State University* Aug. 2011-Aug. 2017

- 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

Research Assistant, *National Taiwan University* Jul. 2007-Jul. 2010

- Fabricated and characterized CIGS and DSSC photovoltaic (PV) devices
- Prepared $CuInSe_2$ thin films by selenizing Cu-In alloy nanoparticles via chemical vapor deposition (CVD) process
- Synthesized ZnO nanospheres and TiO_2 nanotubes via hydrothermal method

Presentations

- "Antimicrobial Properties and Molecular Structures of TSOL"
  Liu, S.-H. et al. *Materials Innovation for Sustainable Agriculture Symposium* **2018**
- "PVP Facilitates {111}-Faceted Au Nanocrystals Formation: Insights from DFT and MD"
  Liu, S.-H. et al. *TechConnect World Innovation Conference* **2015**
- "Shape-Selective Synthesis of Au Nanoparticles: The Role of PVP"
  Liu, S.-H. et al. *AIChE Annual Meeting* **2013**

- "DFT Calculations of the Role of PVP in the Controlled Synthesis of Au Nanostructures" Liu, S.-H. et al. *APS March Meeting* **2013**

Teaching Experience

Teaching Assistant, *The Pennsylvania State University*

CH E 470, Process Design of Chemical Plants — Jan. 2017-May 2017

CH E 524, Molecular Thermodynamics and Statistical Mechanics — Aug. 2016-Dec. 2016

CH E 480, Chemical Engineering Laboratory — Aug. 2015-May 2016

- Demonstrated the unit operations experiments to ~100 undergraduate students
- Taught background theory and data processing on the experiments for ~8 hours a week
- Troubleshot the equipment and resolved the issues with instructors and fellow TAs

CH E 210, Introduction to Material Balances — Jan. 2015-May 2015

CH E 320, Phase and Chemical Equilibria — Aug. 2013-Dec. 2013

Skills

- **Computation:** Python, Linux, Bash, GROMACS, VMD, CHARMM, AutoDock VinaMPI, PDB, MODELLER, Gaussian, VASP, LAMMPS, Simulated Annealing, Machine Learning
- **Synthesis:** CVD, Chemical Reduction, Hydrothermal
- **Characterization:** XRD, SEM, UV-Vis-NIR, Raman, ICP-MS, Solar Simulator

Honors and Awards

- **Oak Ridge Leadership Computing Facility Director's Discretion Project**, *Oak Ridge Leadership Computing Facility* — Dec. 2019
- **Distinguished Conscript**, *Taiwan Air Force* — Aug. 2010-Jul. 2011
- **Presidential Award (Honors)**, *National Taiwan University* — Oct. 2008
- **Undergraduate Research Project**, *Taiwan National Science Council* — Jul. 2007-Feb. 2008