Tao Wei

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Education

- Ph.D., Mork Family Department of Chemical Engineering and Materials Science**,** University of Southern California, 12/2008.
- M.S., Department of Chemical Engineering, Nanjing University of Technology, Nanjing, China, 06/2002.
- B.S., Department of Chemical Engineering, Nanjing University of Technology, Nanjing, China, 06/1999.

Academic Experience

- *Associate Professor*, Dept. of Chemical Engineering and Dept. of Biomedical Engineering, University of South Carolina, 08/2023-present.
- *Associate Professor*, Dept. of Chemical Engineering, Howard University, 2020.
- *Assistant Professor*, Dept. of Chemical Engineering, Lamar University, 2013.
- *Postdoctoral Fellow*, Dept. of Chemical and Biomolecular Engineering, U. of Pennsylvania, 2012-13.
- *Postdoctoral Fellow*, the Dept. of Biomedical Engineering and Materials Research Science and Engineering Center, Northwestern University, 2010-2012.

Awards and Honors

- **NSF CAREER Award, 2020**
- NASA/JPL faculty externship mentor award, 2020
- CEA Faculty Award for excellent research, Howard University, January 2019.
- Chemical Engineering Department Faculty Award **for excellent research and excellent ABET service**, Howard University, February 2019.
- Faculty Fellowship award, Howard University, March 2018.
- "**Jack Gill Faculty Fellow**", Jack Gill Foundation, March 2017.
- Faculty Fellowship award for excellent research and teaching, Lamar University, March 2017.

Research Interests

- Biomaterials (proteins, DNA/RNA, lipids and peptide mimetics) and Bionanotechnologies (biosensors and nanocarrier design for drug delivery) *currently funded by NSF and NASA/JPL*.
- Soft materials (anti-biofouling and fouling release polymers, biopolymers, crosslinked polymer membrane, and semiconducting polymers) *currently funded by ONR and NSF.*
- Nanomaterials and quantum materials (perovskite, 2D materials, zeolites and metal organic frameworks (MOFs) membrane) *currently funded by NSF and DOE.*
- Materials (ceramic and metal alloy) at severe conditions *currently funded by NASA/JPL.*
- Multiscale simulations (quantum, atomistic, coarse-grained and CFD) and machine learning *currently funded by NSF and DOE.*

Media Highlights

- Research projects of surface reactions were reported as a **feature story** in **the annual highlight book** published by **NSF/XSEDE** (the Extreme Science and Engineering Discovery Environment), November 2018. The whole book can be downloaded directly from my webpage: *https://taoweilab.weebly.com/uploads/7/6/0/8/76087311/xsede18_highlights.pdf*
- **Media Highlights** on my project of early cancer detection by Texas Advanced Computer Center and

NSF/Xsede: "Diagnosing Biomarkers in the Bloodstream with a Microscopic Lab-on-a-Chip", June 2017. *https://www.tacc.utexas.edu/-/more-precise-diagnostics-for-better-cancer-outcomes*

- **Media Highlights** on research projects of interfacial phenomena (biosensor development; polymer membrane for water desalination; biointerfacial electron transfer of bio-nano hybrids) by NSF, NSF/Xsede program, and other science websites: "Deep Insights from Surface Reactions", 2016. For example, *https://www.nsf.gov/news/news_summ.jsp?cntn_id=190539&org=NSF&from=news* *https://www.xsede.org/science-successes/-/asset_publisher/lYzwPtSTl56R/content/deep-insights-from-surface-reactions* *https://www.tacc.utexas.edu/-/deep-insights-from-surface-reactions*

Proposals Funded

$4.10 million external grants from NSF, ONR, DoE, NASA, etc.

Publication (* indicates the corresponding author)

(43) Ibrahim Dursun, Maxwell Terban, Yuanze Xu, Xiaoyu Zhang, Sanjit Ghose; Mingxing Li, Pranab Sarker, Hao Li; Mircea Cotlet, **Tao Wei**, Deyu Lu, Qiuming Yu "Temperature-Dependent Optical and Structural Properties of Chiral 2D Hybrid Lead-Iodide Perovskites", *J. Phys. Chem., C* 2023, 127, 31, 15423.

(42) Chi Zhang, Guangle Bu, Md Symon Jahan Sajib, Lida Meng, Shiying Xu, Size Zheng*, Lin Zhang*, **Tao Wei***, "PXLink: A Simulation Program of Polymer Crosslinking to Study of Polyamide Membrane" *Computer Physics Communication*., 2023, 291, 108840.

(41) Pranab Sarker, Tieyi Lu, Di Liu, Guangyao Wu, Hanning Chen, Md Symon Jahan Sajib, Shaoyi Jiang*, Zhan Chen*, **Tao Wei*** "Hydration Behavior of Zwitterionic Materials" *Chemical Science*, 2023, 14, 7500-7511.

(40) Size Zheng, Yong Wei, Yuewei Lin, **Tao Wei***, "Graphic Contrastive Learning Analyses of Discontinuous Molecular Dynamics Simulations: Study of Protein Folding upon Adsorption", *Applied Physics Letters*, 2023, 122, 253701 (**Highlighted with Editor's Picks**).

(39) Grace Tang Chen, Pranab Sarker*, Baofu Qiao*, **Tao Wei***, "Mesoscopic Simulations of Protein Corona Formation on Zwitterionic Peptide-Grafted Gold Nanoparticles" *Journal of Nanoparticle Research*, 2023, 25, 108.

(38) Wen Guo, Tieyi Lu, Satoshi Nagao, **Tao Wei**, Zhan Chen*, "Determine Protein Conformation and Orientation at Buried Solid/Liquid Interfaces", *Chemical Science*, 2023, 14, 2999.

(37) Zhefan Yuan, Patrick McMullen, Sijin Luozhong, Pranab Sarker, Chenjue Tang, **Tao Wei***, Shaoyi Jiang*, "Hidden hydrophobicity impacts polymer immunogenicity", *Chemical Science*, 2023, 14, 2033.

(36) Jie Zheng*, Haspel Nurit*, Liqun Zhang*, **Tao Wei***, Qing Shao*, "Editorial: Computational data-driven design and modeling of biomolecules and biomimetics", *Biophysical Chemistry*, 2022, 289, 106877.

(35) Pranab Sarker, Grace Chen, Md Symon Johan Sajib, Nathan Wesley Jones, **Tao Wei***, "Hydration and Antibiofouling of TMAO-derived Zwitterionic Polymers Surfaces Studied with Atomistic Molecular Dynamics Simulations" *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 2022, 653, 129943.

(34) Jing Chen, Enze Xu, Yong Wei*, Minghan Chen*, **Tao Wei***, Size Zheng*, "Graph Clustering Analyses of Discontinuous Molecular Dynamics Simulations: Study of Lysozyme Adsorption on a Graphene Surface " *Langmuir*, 2022, 38, 35, 10817.

(33) Pranab Sarker, Md Symon Jahan Sajib, Xiuping Tao*, **Tao Wei*** "Multiscale Simulation of Protein Corona Formation on Silver Nanoparticles: Study of Ovispirin-1 Peptide Adsorption" *J. Phys. Chem., B*

2022, 126, 3, 601–608.

(32) Hao Huang, Chengcheng Zhang, Ralph Crisci, Tieyi Lu, Hsiang-Chieh Hung, Md Symon Jahan Sajib, Pranab Sarker, Jinrong Ma, **Tao Wei***, Shaoyi Jiang*, Zhan Chen*, "Strong Surface Hydration and Salt Resistant Mechanism of a New Nonfouling Zwitterionic Polymer Based on Protein Stabilizer TMAO" *J. Am. Chem. Soc.* 2021, 143, 40, 16786–16795.

(31)Wen Guo, Xingquan Zou, Hanjie Jiang, Karl J. Koebke, Marie Hoarau, Ralph Crisci, Tieyi Lu, **Tao Wei***, E. Neil G. Marsh*, Zhan Chen*, "Molecular Structure of Surface Immobilized Super Uranyl Binding Protein" *J. Phys. Chem., B*, 2021, 125, 28, 7706– 7716.

(30) Size Zheng*, Md Symon Jahan Sajib, Yong Wei*, **Tao Wei***, "Discontinuous Molecular Dynamics Simulations of Biomolecule Interfacial Behavior: Study of Ovispirin-1 Adsorption on a Graphene Surface" *J. Chem. Theory Comput*, 2021, 17 (3), 1874–1882

(29) Yi Zuo*, Willam Uspal*, **Tao Wei***, "Airborne Transmission of COVID-19: Aerosol Dispersion, Lung Deposition, and Virus-Receptor Interactions" *ACS Nano*, 2020, 14 (12), 16502.

(28) Yong Wei*, Keith Chin*, Laura M. Barge, Scott Perl, Nino Hermis, **Tao Wei***, "Machine Learning Analysis of the Thermodynamic Responses of In-situ Dielectric Spectroscopy Data in Amino Acids and Inorganic Electrolytes", *J. Phys. Chem., B* 2020, 124, 50, 11491.

(27) Md Symon Jahan Sajib, Pranab Sarker, Yong Wei*, Xiuping Tao*, **Tao Wei***, "Protein Corona on Gold Nanoparticles Studied with Coarse-Grained Simulations", *Langmuir*, 2020, 36, 13356.

(26) Adebola O Adeagbo, **Tao Wei**, Andre Z. Clayborne* "Computational comparative analysis of small atomically precise copper cluster" *J. Phys. Chem., A*, 2020, 6504.

(25) Md Symon Jahan Sajib, Ying Wei, Ankit Mishra, Lin Zhang, Ken-ichi Nomura, Rajiv K. Kalia, Priya Vashishta, Aiichiro Nakano*, Sohail Murad*, **Tao Wei***, "Atomistic Simulations of Biofouling and Molecular Transfer of Crosslinked Aromatic Polyamide Membrane for Desalination", *Langmuir*, 2020, 36, 7658.

(24) Mohammadreza Samieegohar, Feng Sha, Andre Z. Clayborne, **Tao Wei***, "Peptide-grafted gold nanoparticles studied with ReaxFF MD simulations", *Langmuir* 2019, 35, 5029.

(23) **Tao Wei***, Chulai Ren*, "Theoretical Simulation Approaches to Polymer Research" In *Polymer Science and Innovative Applications*, pp. 207-228, Eds. Elsevier.

(22) Ivan Guerrero*, Enrique Gonz´alez-Tovar, Mart´ın Ch´avez-P´aez, **Tao Wei**, "Expansion and shrinkage of the electrical double layer in charge-asymmetric electrolytes: A non-linear Poisson-Boltzmann description", *Journal of Molecular Liquids* 2019, 277, 104-113.

(21) Nicholas P. van der Munnik, Md Symon Jahan Sajib, Melissa A. Moss, **Tao Wei**, Mark J. Uline "Determining the potential of mean force for Amyloid-β dimerization: combining self consistent field theory with molecular dynamics simulation", *J. Chem. Theory Comput.* 2018, 14, 2696.

(20) Tony Yen, Xin Fu, **Tao Wei**, Roshan Nayak, Yuesong Si, Yu-Hwa Lo "Reversing Coffee-Ring Effect by Laser-Induced Differential Evaporation", *Scientific Reports*, 2018, 8, 3157.

(19) Md Symon Jahan Sajib, Mohammadreza Samieegohar, **Tao Wei***, Katherine Shing*, "Atomic-level simulation study of n-hexane pyrolysis on silicon carbide surfaces", *Langmuir*, 2017, 33 (42), 11102-11108. (**Selected as Journal Featured Article**)

(18) Mohammadreza Samieegohar, Heng Ma, Feng Sha, Md Symon Jahan Sajib, Ivan.Guerrero, **Tao Wei***, "Understanding the interfacial behavior of lysozyme on Au (111) surfaces with multiscale simulations". *Applied Physics Letters* 2017, 110 (7), 073703.

(17) Tiantian Zhang, **Tao Wei**, Yuanyuan Han, Heng Ma, Mohammadreza Samieegohar, Ping-Wei Chen,

Ian Lian, Yu-Hwa Lo, "Transient induced molecular electronic spectroscopy (TIMES) for protein-ligand interaction detection: experimental and theoretical studies", *ACS Central Science* 2016, 2 (11), 834. (**Selected as Journal Featured Article**) (**Media Highlights**)

(16) **Tao Wei***, Lin Zhang, Haiyang Zhao, Heng Ma, Sohail Murad*, "Aromatic polyamide reverse osmosis membrane: an atomistic molecular dynamic simulation" *J. Phys. Chem. B* 2016, 120, 10311. (**Media Highlights**)

(15) **Tao Wei***, Heng Ma, Aiichiro Nakano*, "Decaheme cytochrome MtrF adsorption and electron transfer on gold surface". *J. Phys. Chem., Letters* 2016, 7, 929. (**Media Highlights**)

(14) **Tao Wei***, Md Symon Jahan Sajib, Mohammadreza Samieegohar, Heng Ma, Katherine Shing*, "Self-assembled monolayers of azobenzene derivative on silica and their interactions with lysozyme", *Langmuir* 2015, 31 (50), 13543.

(13) C. Masato Nakano, Erick Moen, Hye Suk Byun, Heng Ma, Bradley Newman, Alexander McDowell, **Tao Wei***, and Mohamed Y. El-Naggar*, "iBET: immersive visualization of biological electron-transfer dynamics", *Journal of Molecular Graphics and Modelling* 2016, *65*, 94.

(12) C. Masato Nakano, Md Symon Jahan Sajib, Mohammadreza Samieegohar, **Tao Wei***, "Field-induced stacking transition of biofunctionalized trilayer graphene". *Applied Physics Letters* 2015, 108, 051601.

(11) Yubiao Niu, Tiefan Huang, Zhijun Zhou, Guohua Xu, Lin Zhang, **Tao Wei**, "Formation of cyclodextrin monolayer through a host-guest interaction with tailor-made phenyltriethoxysilane self-assembled monolayer", *Colloids and Surfaces A* 2015, 470, 224.

(10) Masato Nakano, Heng Ma, **Tao Wei***, "Study of lysozyme mobility and binding free energy during adsorption on a graphene surface", *Applied Physics Letters* 2015, 106, 153701.

(9) C. Masato Nakano, Hye Suk Byun, Heng Ma, **Tao Wei***, Mohamed Y. El-Naggar, "A framework for stochastic simulations and visualization of biological electron-transfer dynamics", *Computer Physics Communications* 2015, 193, 1.

(8) **Tao Wei***, Tiefan Huang, Baofu Qiao, Mo Zhang, Heng Ma, Lin Zhang, "Structures, dynamics and water permeation free energy across bilayers of lipid A and its analog studied with molecular dynamics simulation", *J. Phys. Chem. B* 2014, 118, 13202.

(7) **Tao Wei**, Marcelo A. Carignano, Igal Szleifer, "Molecular dynamics simulation of lysozyme adsorption/desorption on hydrophobic surfaces", *J. Phys. Chem. B* 2012, 116 (34), 10189.

(6) **Tao Wei**, Marcelo A. Carignano, Igal Szleifer, "Lysozyme adsorption on polyethylene surfaces: why are long time simulations needed?", *Langmuir* 2011, 27(19), 12074.

(5) **Tao Wei**, Sarawut Kaewtathip, Katherine Shing, "Buffer effect on protein adsorption at liquid/solid interface", *J. Phys. Chem. C* 2009, 113 (6), 2053.

(4) **Tao Wei**, Shengjing Mu, Aiichiro Nakano, Katherine Shing, "A hybrid multi-loop genetic-algorithm/simplex/ spatial-grid method for locating the optimum orientation of an adsorbed protein on a solid surface", *Computer Physics Communications* 2009, 180 (5), 669.

(3) Hongbin Lu, Hongbin Shen, Zhenlun Song, Katherine Shing, **Tao Wei**, Steven Nutt, "Rodlike silicate-epoxy nanocomposites", *Macromolecular Rapid Communications* 2005, 26 (18), 1445.

(2) Chang Liu, Xin Feng, Xiaoyan Ji, Dongliang Chen, **Tao Wei**, Xiaohua Lu, "The study of dissolution kinetics of K_2SO_4 crystal in aqueous ethanol solutions with a statistical rate theory", *Chinese Journal of Chemical Engineering* 2004, 12 (1), 128.

(1) Xiaoyan Ji, Dongliang Chen, **Tao Wei**, Xiaohua Lu, Yanru Wang, Jun Shi, "Determination of dissolution kinetics of K_2SO4 crystal with ion selective electrode", *Chemical Engineering Science* 2001, 56, 7017.

Conference Presentations and Proceedings

(52) Ken-ichi Nomura, Aiichiro Nakano, Priya Vashishta, Pratibha Dev, **Tao Wei**, "CyberMAGICS: Cyber Training on Materials Genome Innovation for Computational Software for Future Engineers", ASEE conference, 2023

(51) Pranab Sarker, Grace Tang Chen, Md Symon Jahan Sajib, Nathan Wesley Jones, **Tao Wei**, "Atomistic modeling of hydration and antibiofouling of TMAO-polymer surfaces", APS spring conference, 2023 (accepted)

(50) Pranab Sarker, **Tao Wei**, "Understanding Strong Hydration, Salt-Resistance, and Antibiofouling of Zwitterionic Materials from Ab Initial Simulations", APS spring conference, 2022.

(49) C. Psarakis, S. D. Vance, A. Kavner, K. Chin, T. T. Fidelis, P. Sarker, **T. Wei**, B. Journaux, M. J. Styczinski, A. Solomonidou, "Electrical Properties of Ocean Worlds:Laboratory and Computational Investigations", Lunar and Planetary Science Conference, 2022.

(48) **Tao Wei**, "Hydration and Antibiofouling of Zwitterionic Polymers Studied with Quantum and Atomistic Simulations", Pacifichem 2021.

(47) **Tao Wei**, "Multiscale Simulation of Protein Corona Formation on Metal Nanoparticles", Pacifichem 2021.

(46) Pranab Sarker, Md Symon Jahan Sajib, **Tao Wei**, "Ab Initio Molecular Dynamics Simulations of the Hydration of Zwitterions", AICHE Fall Meeting, 2021.

(45) Md Symon Jahan Sajib, Pranab Sarker, Xiuping Tao, **Tao Wei**, "Protein Corona Formation Studied with Multiscale Simulations" AICHE Fall Meeting, 2021.

(44) **Tao Wei**, "Simulation Studies of Zwitterionic Materials for Antibiofouling from Quantum and Atomistic Scales", AICHE Fall Meeting, 2021.

(43) **Tao Wei**, "Atomistic Simulations of Aromatic Polyamide Membrane", AICHE Fall Meeting, 2021.

(42) Pranab Sarker, Symon Sajib, **Tao Wei**, "Quantum Dynamics and Atomistic Molecular Dynamics Simulations of Zwitterionic TMAO Surface's Hydration and Antibifouling", *ACS Spring National Meeting*, 2021.

(41) Md Symon Jahan Sajib, Ying Wei, Ankit Mishra, Lin Zhang, Ken-Ichi Nomura, Rajiv K. Kalia,Priya Vashishta, Aiichiro Nakano, Sohail Murad, **Tao Wei**, "Atomistic Simulations of Biofouling and Molecular Transfer of a Cross-linked Aromatic Polyamide Membrane for Desalination", *ACS Spring National Meeting*, 2021.

(40) Chi Zhang, Md Symon Jahan Sajib, Guangle Bua,Lida Meng, Shiying Xu, Size Zheng, Lin Zhang, **Tao Wei**, "Atomistic molecular dynamics simulations of polymer membrane crosslinking and surface modifications", *ACS Spring National Meeting*, 2021.

(39) Md Symon Jahan Sajib, Pranab Sarker, Yong Wei, Xiuping Tao, **Tao Wei**, "Understanding Protein Corona Formation from Coarse-Grained and Atomistic Molecular Dynamics", *ACS Spring National Meeting*, 2021.

(38) Samentha Dumervil, Steve Vance, Keth Chin, **Tao Wei**, "Electrical Conductivity and Magnetic Induction on Europa", *AGU Fall National Meeting*, San Francisco, 2020.

(37) Merina Jahan, Heng Ma, Mark Uline, **Tao Wei**, "Atomistic Simulation and Molecular Field Theory Study of DNA Hybridization in Self-Assembling Monolayer Surfaces", *AICHE Fall National Meeting*, Orlando, 2019.

(36) Size Zheng, Ying Wei, Chidumebi Alim, Eliel Akinbami, Md Symon Jahan Sajib, **Tao Wei** "Formation of Protein Corona on A Gold Nanoparticle Studied with Discontinuous Molecular Dynamics and

Atomistic Molecular Dynamics Simulations", *AICHE Fall National Meeting*, Orlando, 2019.

(35) Md Symon Jahan Sajib, **Tao Wei**, "Molecular Understanding of Polyamide Membrane in Desalination at Equilibrium and Nonequilibrium States Using Molecular Simulations", *AICHE Fall National Meeting*, Orlando, 2019.

(34) Md Symon Jahan Sajib, William Jean-Baptiste, Keith Chin, **Tao Wei** "Interfacial Behavior of Amino Acid Residues on Gold Surfaces Studied with Electrical Spectroscopy and Atomistic ReaxFF Simulations" *ACS Fall National Meeting,* San Diego, 2019.

(33) K. Chin, **T. Wei**, N. Hermis, J. Pasalic, S. Perl, L. M. Barge, "Electrochemical Properties Characterization of Planetary Analogues by Electrical Spectroscopy", *Astrobiology Science Conference*, Seattle, 2019.

(32) **Tao Wei**, "Interactions of Gold Nanoparticles with Phospholipid Bilayer Studied with Coarse-grained Molecular Dynamics Simulations", *ACS Spring National Meeting,* Orlando, 2019.

(31) **Tao Wei**, "Peptide-grafted gold nanoparticles studied with ReaxFF MD simulations", *ACS Fall National Meeting*, Boston, 2018.

(30) **Tao Wei**, "Silicon Carbide Surfaces for Pyrolysis Studied with ReaxFF MD Simulations", *ACS Spring National Meeting*, New Orleans, 2018.

(29) Nicholas P. van der Munnik, Kathleen Mingle, **Tao Wei**, Jochen Lauterbach, Mark J. Uline, Melissa A. Moss "Polyacid-Functionalized Gold Nanoparticles As an Amyloid-β Inhibitor Platform", *AICHE Fall National Meeting*, Minneapolis, 2017.

(28) M. S. J. Sajib, **T. Wei** "A Non-Equilibrium Molecular Dynamics (NEMD) Simulation of the Crosslinked Polyamide Membranein Water Desalination", *AICHE Fall National Meeting*, Minneapolis, 2017.

(27) Md Symon Jahan Sajib, **Tao Wei** "Molecular simulations of reverse osmosis aromatic polyamide membrane: mechanical properties, desalination, crosslinking degree and monomers' isomer", *AICHE Fall National Meeting*, San Francisco, 2016.

(26) Heng Ma, **Tao Wei** "Study of ion behavior, morphology and hybridization on DNA self assemble membrane via molecular dynamics" *AICHE Fall National Meeting*, San Francisco, 2016.

(25) Nicholas P. van der Munnik, Symon Sajib, **Tao Wei**, Melissa A. Moss and Mark J. Uline "Statistical thermodynamic modeling of early Amyloid-β oligomer formation: explicit and implicit incorporation of hydrogen bonding in a self-consistent field framework", *AICHE Fall National Meeting*, San Francisco, 2016.

(24) Mohammadreza Samieegohar, **Tao Wei**, "Protein interfacial behavior studied with multiscale simulations", *AICHE Fall National Meeting*, San Francisco, 2016.

(23) **Tao Wei**, "Biohybrid of multi-heme cytochrome and surfaces of Au and graphene: protein adsorption and electron transfer", *ACS Fall National Meeting*, Philadelphia, 2016.

(22) Mohammadreza Samieegohar, **Tao Wei**, "Multiscale simulation of proteins' motion in a microchannel", *AIChE Spring National Meeting*, Houston, 2016.

(21) Tiantian Zhang, Heng Ma, Ian Lian, **Tao Wei**, Yu-Hwa Lo, "Development of transient induced Molecular Electronic Spectroscopy (TIMES) for protein-ligand interactions", *ACS Spring National Meeting*, San Diego, 2016. (**Best Presentation Award in 251th ACS conference**)

(20) Heng Ma, Md. Symon Sajib, **Tao Wei**, "Adsorption and electron transfer of deca-heme cytochrome (MtrF) studied with atomistic simulations and kinetic Monte Carlo simulation", *ACS Spring National Meeting*, San Diego, 2016.

(19) Hye Suk Byun, C. Masato Nakano, Heng Ma, **Tao Wei**, Mohamed Y. El-Naggar, "Divide-conquer-

recombine kinetic Monte Carlo simulations of electron transfer in the extracellular redox network of *Shewanella oneidensis* MR-1", *Biophysical Society Spring Meeting*, Los Angeles, 2016.

(18) Heng Ma, C. Masato Nakano, Hye Suk Byun, Mohamed Y. El-Naggar, **Tao Wei**, "Adsorption and electron transfer of bacterial decaheme cytochrome Mtrf on gold surface studied with atomistic molecular dynamics simulation, free energy computation and kinetic Monte Carlo simulation", *AIChE Fall National Meeting*, Salt Lake City, 2015.

(17) Mohammadreza Samieegohar, **Tao Wei**, Ian Lian, Liangbiao Chen, "The fluidization and adsorption of soft particles studied with hybrid element method and fluid dynamics", *AIChE Fall National Meeting*, Salt Lake City, 2015.

(16) Nicholas P. van der Munnik, **Tao Wei**, Melissa A. Moss, Mark J. Uline, "Statistical thermodynamics of Amyloid-β Oligomerization", *AIChE Fall National Meeting*, Salt Lake City, 2015.

(15) Heng Ma, Ian Lian, **Tao Wei**, "DNA Hybridization on silica surface for gene chip design studied with molecular dynamics simulations", *AIChE Spring National Meeting*, Austin, 2015.

(14) Symon Sajib, **Tao Wei**, Katherine Shing, "Lysozyme adsorption and desorption on the azobenzene self-assembling surfaces studied with molecular dynamics simulations", *AIChE Spring National Meeting*, Austin, 2015.

(13) Heng Ma, **Tao Wei**, "Structures, dynamics, and water permeation free energy across bilayers of Lipid A and its analog studied with molecular dynamics simulation", *AIChE Spring National Meeting*, Austin, 2015.

(12) **Tao Wei**, Katherine Shing, "Interactions of lysozyme and azobenzene derivatives in the solution and on a surface", *APS Spring National Meeting*, San Antonio, Spring 2015.

(11) Heng Ma, Haiyang Zhao, Lin Zhang, **Tao Wei**, "Atomistic modeling of cross-linked polyamide/graphene and polyamide/graphene oxide composites reverse osmosis membrane", *AIChE Fall National Meeting*, Atlanta, 2014.

(10) Haiyang Zhao, **Tao Wei**, Lin Zhang, "Water permeability of polyamide/graphene and polyamide/graphene oxide composites reverse osmosis membrane studied with atomistic simulations",*ACS Fall National Meeting*, San Francisco, 2014

(9) **Tao Wei**, Robert Riggleman, "Phase behavior of rod-coil block copolymers in the melt and at fluid interfaces", *AIChE Fall National Meeting*, San Francisco, 2013.

(8) **Tao Wei**, Robert Riggleman, "Phase behaviors of rod-coil block copolymer in three dimension studied by Monte Carlo simulations", *APS Spring National Meeting*, Baltimore, Spring 2013.

(7) **Tao Wei**, Mo Zhang, Lin Zhang, "Atomistic modeling of lipid A and its analogue supramolecular bilayer assembly in solution", *ACS Spring National Meeting, Philadelphia*, Spring 2012.

(6) Feng Sha, Ying Wei, **Tao Wei**, "Parallel molecular dynamics simulation of lysozyme hydration on IBM blade center cluster", *Proceeding of IEEE International Conference on Intelligent Computing and Intelligent Systems*, 2010, 2, 479-482.

(5) **Tao Wei**, Marcelo A. Carignano, Igal Szleifer, "Hydration and structural deformation of lysozyme upon adsorption on a polyethylene surface studied by molecular dynamics simulation", *ACS Spring National Meeting, Anaheim*, Spring 2011.

(4) **Tao Wei**, Wei Chen, "Non-equilibrium molecular dynamics simulation study of the transport of pure CO_2 and CO_2/CH_4 mixture through nanopore the framework of zeolites (MFI and LTA) and metal-organic frameworks (Cu-BTC)", *ACS Spring National Meeting,* San Francisco, Spring 2010.

(3) **Tao Wei**, Shengjing Mu, Aiichiro Nakano, Katherine Shing, "Locating optimum orientations of adsorbed

protein on a solid surface using a hybrid genetic algorithm and spatial grid method", *AIChE Spring National Meeting,* New Orleans, Spring 2008.

(2) **Tao Wei**, Sarawut Kaewtathip, Katherine Shing, "Buffer effect on protein adsorption on solid surfaces", *ACS National Meeting,* New Orleans, Spring 2008.

(1) **Tao Wei**, Sarawut Kaetathip, Katherine Shing, "Adsorption kinetics and secondary structure of IgG adsorbed on solid surfaces", *ACS National Meeting*, San Diego, Spring 2003.

Recent Invited Talks

(21) "Multiphysics and multiscale simulation methods for electromagnetic energy assisted fossil fuel to hydrogen conversion", Crosscutting Research – University Training Camp; Research Program, DOE, Nov, 2021.

(20) "Simulation Studies of Antibiofouling Zwitterionic Polymer Surfaces", Office of Naval Research (ONR) Antifouling & Fouling Release Coatings Program Review, Nov. 2021.

(19) "Simulations of Materials Interfacial Reactions". Chemistry Department, Stony Brook University, Feb., 2021

(18) "Simulation Studies of Zwitterionic and Amphiphilic Surfaces for Antibiofouling and Fouling Release", Office of Naval Research (ONR) Antifouling & Fouling Release Coatings Program Review, Nov. 2020.

(17) "Simulation Studies of Surface-Modified Polyamide-Nanoparticle (Iron Oxide and Graphene Oxide) Composite Membrane for Water Treatment", NSF meeting of U.S.-Africa Collaborations: Nanoscale Interactions and Nanotechnology Convergence, Oct, 2020.

(16) " Simulations Studies of Surface Reactions", the Department of Chemical and Biomolecular Engineering, University of Maryland, College Park, Sept, 2020.

(15) "Biomaterials and Polymer Membrane Design Using Multiscale Simulations (Quantum, Atomistic and Coarse-grained)", Depart. of Electrical Engineering and Computer Science, Howard University, 2020

(14) "Computer Simulations for Biointerfaces and Biosensor Design", *Biochemistry and Molecular Biology Department*, Howard University, 2020.

(13) "Atomistic molecular simulations of polyamide membrane in desalination at equilibrium and nonequilibrium states", NSF-funded *US-Africa Forum on Nanotechnology Convergence for Sustainable Energy, Water and Environment, Johannesburg*, South Africa, 2019.

(12) "Multiscale simulations of extracellular electron transfer across multiple-heme proteins", NSF-funded *US-Africa Forum on Nanotechnology Convergence for Sustainable Energy, Water and Environment*, Johannesburg, South Africa, 2019.

(11) "Simulations of crosslinked polymer membrane and semiconducting polymers", NIST, July, 2019.

(10) "Water diffusive behavior inside polymer membrane, across lipid layers and on protein surfaces", NIH, March, 2019.

(9) "Atomistic simulations and Statistical Mechanics in materials research", the Chemistry Department at Howard University, February, 2019.

(8) "Biointerfacial behavior and biosensing", NASA/JPL, January, 2019.

(7) "Reactive forcefield simulations of pyrolysis on silicon carbide surfaces and chemical reactions at the bio-nano interface", the Department of Mechanical & Aerospace Engineering at the University of the George Washington University, DC, March, 2018.

(6) "Study of protein interfacial phenomena and its applications in biotechnology", *National Forum of the*

Functional Nano-materials and Interface, Su Zhou, China, 2017.

(5) "Study of Biointerfacial Phenomena for Applications in Functional Materials and Biotechnologies", Southeast University, China, 2017.

(4) "Studies of interfacial phenomena for applications in biotechnologies and water treatment", the Physics Department at Trinity University, Texas, 2017.

(3) "Electron transfer and adsorption of proteins on surfaces", Institute of Physics, the Autonomous University of San Luis Potosí, México, 2016.

(2) "Molecular simulations of bio-interfacial phenomena for applications in sustainable energy", ENN Energy Research Institute, China, January 2016.

(1) "Computer simulations of bio-interface for functional materials design", Department of Chemical and Biological Engineering, Zhejiang University, China, 2016.

Student Theses and Dissertations

(5) Md Symon Jahan Sajib, PhD, November, 2017, "Atom-level simulation study of interfacial interactions: self-assembling monolayer surfaces, silicon carbide ceramic materials and polymer membrane".

(4) Tejus Mane, Master Thesis, July, 2017, "Understanding Teracycline Stricture's Role in Promoting Anti-inflammatory Response Using Atomistic Simulation, Docking Analysis and Creative Synthesis".

(3) Mohammadreza Samieegohar, PhD Dissertation, July 2017, "Molecular Understanding of Biointerfacial Behavior for Biosensing and High-Temperature Interfacial Chemical Reactions in Pyrolysis".

(2) Heng Ma, PhD Dissertation, July, 2017, "Biointerfacial Phenomena: Water Permeation, Protein adsorption, Electron Transfer and DNA Hybridization".

(1) Mohammadreza Samieegohar, Master Thesis, Dec. 2015, "Multiscale Modeling and Simulation of Proteins Motion in the Microchannel".

Teaching Experience

08/2017-present: Department of Chemical Engineering, Howard University

- *Thermodynamics* (graduate course).
- *Thermodynamics* (undergraduate course).
- *Chemical Engineering Analysis* (undergraduate course).
- *Chemical Engineering Design* (undergraduate course).
- *Unit Operation Lab* (undergraduate course).

09/2013-08/2017: Department of Chemical Engineering, Lamar University

- *Thermodynamics I* (undergraduate course).
- *Thermodynamics II* (undergraduate course).
- *Heat Transfer* (undergraduate course).
- *Statistical Mechanics / Thermodynamics* (graduate course).
- *Soft Matter Simulations* (graduate course).
- *Materials Modeling and Simulations* (graduate course).

Professional Affiliation

- American Chemical Society (ACS);
- American Institute of Chemical Engineers (AICHE);
- American Physical Society (APS);
- Sigma Xi (Senior Member)
- Biophysical Society (BPS)

Service

Organize Conferences, Workshops and Journal Publications

- Chair for the session in DCOMP, "Emerging Trends in Molecular Dynamics and Machine Learning", APS, spring, 2021.
- Chair/Co-Chair for the session "Dynamics and Modeling of Particles, Crystals and Agglomerate Formation" at AICHE national meeting, San Francisco, fall 2020; Pittsburgh, fall 2018; Minneapolis, fall 2017; San Francisco, fall 2016.
- Organized NSF-funded bionanotechnology summer workshop, D.C. Washington, 2019-2021.
- Panelist for the NSF-supported US-Africa Forum on Nanotechnology Convergence for Sustainable Energy, Water and Environment", Johannesburg, South Africa, August 2019.
- Chair for the session of "Basic Research in Colloids, Surfactants & Interfaces" of the Division of Colloid and Surface Chemistry. ACS National Conference, San Diego, fall 2019; Orlando, spring 2019.
- Chair for the session of "Lipids, Peptides & Proteins" at the Division of "Division of Colloid and Surface Chemistry" in ACS national conference, Boston, fall 2018.
- Co-organized DOE-funded Materials Simulation Workshop, Gaithersburg, Nov. 2018.
- Co-chair for the session of "Modeling and Simulation of Composites" at AICHE national meeting, Atlanta, fall 2014.
- Serve as a guest editor for Special Issue in Biophysical Chemistry, 2021.

Review Proposals and Manuscripts

- Serving as a panelist for NSF proposal review, 2016-2023.
- Proposal review for ACS Petroleum Research Fund, 2021-2022.
- Reviewer for 30 journals in Chemistry, Physics, Bioengineering and Chemical Engineering: JACS, ACS Nano, ACS Central Science, Langmuir, Soft Matter, Biointerphases, J. Phys. Chem. (A, B, C), J. Chem. Phys., Fuel & Energy, Appl. Phys. Lett., J. Colloid Interface Sci., Comput. Phys. Commun., AICHE, etc.
- Serving on Doctoral Dissertation and Master's Theses Committees for 38 graduate students from Chem. Eng. Dept. and Mathematics Dept. at Lamar University and Howard University.

Service to the Profession and Department/College/University

- Advisor for AICHE Chapter, Howard University.
- Committee chair of faculty participating research, College of Engineering and Architecture, Howard U.
- Member of student grievance committee, College of Engineering and Architecture, Howard U.
- Member of the department APT (Appointments, Promotion and Tenure) committee, Howard U.
- Severing as a secretary for National Capital Section (NCS) of AIChE.