

## Tao Wei

Associate Professor, Department of Biomedical Engineering, Department of Chemical Engineering,  
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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, 2020-23.
- *Assistant Professor*, Dept. of Chemical Engineering, Lamar University, 2013-17.
- *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, 2010-12.

### Awards and Honors

- **NSF CAREER Award, 2020**
- NASA/JPL faculty externship mentor award
- 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](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.nsf.gov/news/news_summ.jsp?cntn_id=190539&org=NSF&from=news)

### **Proposals Funded**

**\$4.21 million total; (\$3.52 million as PI; \$3.35 as a single PI)** from NSF, ONR, DoE, NASA, etc.

### **Publication** (\* indicates the corresponding author)

- (52) Qinyi Fu, Nisha Verma, Ruipeng Li, Masafumi Fukuto, Size Zheng, Roberto Gambarini, **Tao Wei\***, Benjamin Ocko\*, Benjamin S. Hsiao\*, "Grazing Incidence Wide-Angle X-ray Scattering of Water Adsorption in Solvent-Modified Polyamide Barrier Layers of Reverse Osmosis Membranes", *Macromolecules*, 2024, (Accepted)
- (51) Xiaoxue Qin, Jiahuiyu Fang, Ariana Annie Chen, Pranab Sarker, Md Symon Johan Sajib, Mark J. Uline\*, **Tao Wei\***, "Hydration and Antibiofouling Behavior of Zwitterionic Polycarboxybetaine-Grafted Surfaces Studied with Atomistic Simulations", 2024, *Langmuir*, 2024, (Accepted)
- (50) Size Zheng, Jacob Gissing, Benjamin S. Hsiao\*, **Tao Wei\***, "Interfacial Polymerization of Aromatic Polyamide Reverse Osmosis Membranes", *ACS Applied Materials & Interfaces*, 2024, 16, 65677.
- (49) Chen Chen, Enze Xu, Defu Yang, Haibing Yin, **Tao Wei\***, Hanning Chen\*, Yong Wei\*, Minghan Chen\*, "Chemical Environment Adaptive Learning for Optical Band Gap Prediction of Doped Graphitic Carbon Nitride Nanosheets", *Neural Computing and Applications*, 2024, 1-15.
- (48) Xiaoxue Qin, Ariana Annie Chen, Jiahuiyu Fang, Pranab Sarker, Mark J. Uline\*, **Tao Wei\***, "Atomistic Simulations of Hydration and Antibiofouling Behavior of Amphiphilic Polymer Brush Surfaces Functionalized with TMAO and Short Fluorocarbon", *Langmuir*, 2024, 40, 23994.
- (47) Hao Li, Pranab Sarker, Xiaoyu Zhang, Maxwell W. Terban, Sanjit Ghose, Ibrahim Dursun, Mircea Cotlet, Mingxing Li, Yugang Zhang, Yuanze Xu, Shripathi Ramakrishnan, **Tao Wei**, Deyu Lu, Qiuming Yu\*, "Enhancing chiroptoelectronic activity in chiral 2D perovskites via chiral-achiral cation mixing", *Advanced Optical Materials*, 2024, 2401782.
- (46) Catherine A. Psarakis\*, Timothy Tizhe Fidelis, Keith B. Chin, Baptiste Journaux, Abby Kavner, Pranab Sarker, Marshall J. Styczinski, Steven D. Vance, **Tao Wei**, "Electrical Conductivity of Subsurface Ocean Analogue Solutions from Molecular Dynamics Simulations", *ACS Earth Space Chem.*, 2024, 8, 1146.
- (45) Yuchen Wu, Ting Lin, Elizabeth Santos, Dongchan Ahn, Ryan Marson, Pranab Sarker, Xiaoyun Chen, Frédéric Gubbels, Nick E. Shephard, Carol Mohler, **Tao Wei\***, Tzu-Chi Kuo\*, Zhan Chen\*, "Molecular Behavior of Silicone Adhesive at Buried Polymer Interface Studied by Molecular Dynamics Simulation and Sum Frequency Generation Vibrational Spectroscopy", *Soft Matter*, 2024, 20, 4765.
- (44) Yong Wei, Amy X. Chen, Yuewei Lin, **Tao Wei\***, Baofu Qiao\*, "Allosteric Regulation in SARS-CoV-2 Spike Protein", *Phys. Chem. Chem. Phys.*, 2024, 26, 6582-6589. (**Selected as "2024 HOT PCCP article"**)
- (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, Shiyong 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, Tiewei 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. (**Selected as "2023 Chemical Science HOT Article Collection"**)
- (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, Tiewei 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, Tiewei 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. (**Ranks as one of "JACS most cited publications from 2020-2021"**)
- (31) Wen Guo, Xingquan Zou, Hanjie Jiang, Karl J. Koebke, Marie Hoarau, Ralph Crisci, Tiewei 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- $\beta$  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<sub>2</sub>SO<sub>4</sub> 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<sub>2</sub>SO<sub>4</sub> crystal with ion selective electrode", *Chemical Engineering Science* 2001, 56, 7017.

### **Conference Presentations and Proceedings**

- (61) Pranab Sarker, Jiahuiyu Fang, Shuting Zhang, **Tao Wei**, "Interactions and kinetics of electron Transfer between an iron oxide nanoparticle and Shewanella oneidensis cytochromes", *MRS fall conference*, Boston, 2024. (Invited Talk)
- (60) Jiahuiyu Fang, Shuting Zhang, Pranab Sarker, Xiaoxue Qin, Roberto Gambarini, Mark Uline, Aiichiro Nakano, **Tao Wei**. "Adsorption and Electron Transfer Behaviors of Decaheme Cytochrome Protein MtrF on Ion Oxide Nanoparticle Surfaces", *ACS Fall Conference*, Denver, 2024.
- (59) Xiaoxue Qin, Ariana Chen, Jiahuiyu Fang, Pranab Sarker, Mark J. Uline, **Tao Wei**, "Atomistic Study on the Hydration and Fouling Resistance Behaviors of Hybrid Amphiphilic and Zwitterionic Polymer Surfaces", *ACS Fall Conference*, 2024.
- (58) Roberto Gambarini, Size Zheng, Mark Uline, **Tao Wei**, "Molecular interactions of PFAS on Polyamide Membranes using Atomistic Molecular Dynamics Simulations", *ACS Fall Conference*, 2024.
- (57) Size Zheng, **Tao Wei**, Benjamin Hsiao, "Interfacial Polymerization of Aromatic Polyamide Reverse Osmosis Membrane", *ACS Fall Conference*, 2024.
- (56) **Tao Wei**, "Surface Hydration and Fouling Resistant Behaviors of Zwitterionic Polymers" *ACS Fall*

*Conference*, 2024. (Invited Talk)

- (55) **Tao Wei**, "Simulation Study of Hydration and Nonfouling Activities Zwitterionic Materials", 5th International Conference on Bioinspired and Zwitterionic Materials, Cornell University (Invited Talk).
- (54) **Tao Wei**, "Simulation Studies of Antibiofouling Zwitterionic materials", *Pittcon Spring Conference*, 2024. (Invited Talk)
- (53) Yuchen Wu, Ting Lin, Elizabeth Santos, Dongchan Ahn, Ryan Marson, Pranab Sarker, Xiaoyun Chen, Gubbels, Frederic, Chris Tucker, Nick E. Shephard, Carol Mohler, **Tao Wei**, Tzu-Chi Kuo, Zhan Chen, "Probing Molecular Behavior of Silicone Adhesives at Buried Interfaces in Situ Using Sum Frequency Generation Vibrational Spectroscopy and Molecular Dynamics Simulation", *Adhesion Society Spring Conference*, 2024.
- (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.
- (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", Pacificchem 2021.
- (47) **Tao Wei**, "Multiscale Simulation of Protein Corona Formation on Metal Nanoparticles", Pacificchem 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, Shiyong 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- $\beta$  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 Membrane in 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- $\beta$  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- $\beta$  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<sub>2</sub> and CO<sub>2</sub>/CH<sub>4</sub> 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**

- (26) Tao Wei, "Materials Interfaces: Fouling Resistance and Interfacial Redox", Chemistry Department, *University of Missouri, Columbia*, September 2024.
- (25) Tao Wei, "Surface Hydration and Fouling Resistant Behaviors of Zwitterionic Polymers" *ACS Fall Conference*, August, 2024.
- (24) Tao Wei, "Simulation Studies of New Zwitterionic and Amphiphilic Materials", *Office of Naval Research (ONR)*, Ithaca, June, 2024.
- (23) Tao Wei, "Materials Interfaces and Applications", Physics Department, *University of North Carolina, Charlotte*, May, 2024
- (22) “Simulation Studies of Antibiofouling Zwitterionic materials”, *Pittcon Spring Conference*, 2024.
- (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**

#### **01/2024-present: Department of Biomedical Engineering, University of South Carolina**

- *Thermodynamics of Biomolecular Systems* (undergraduate course).
- *Modeling & Simulation of Biomedical System* (graduate course)

#### **08/2017-05/2023: 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);
- Biophysical Society (BPS);
- Sigma Xi (Senior Member)

**Service**

***Organize Conferences, Workshops and Journal Publications***

- Organized the symposium, “Recent Development of Polymer Interface and Polymer Thin Film Preparation, Characterization, and Modeling”, ACS fall conference, 2024.
- 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, 2016-2024.
- Serving as a panelist for DoE proposal review, 2022-2023.
- 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 40 graduate students from Chem. Eng. Dept. and Mathematics Dept. at Lamar University and Howard University.

***Service to the Profession and Department/College/University***

- Mentoring REU students in the summer of 2022-23, U. of South Carolina
- 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.
- Serving as a secretary for National Capital Section (NCS) of AIChE.