Zhenghao Wu

EMPLOYMENT

Xi'an Jiaotong-Liverpool University *China, June. 2023 - Present*
Assistant Professor at Department of Chemistry

Northwestern University *United States, Nov. 2021 - May 2023*
Postdoctoral Fellow at Department of Civil and Environmental Engineering

- Advisor: **Prof. Sinan Keten**

EDUCATION

Technische Universität Darmstadt *Germany, Aug. 2018 - Oct. 2021*
Dr. rer. nat. in Theoretical Chemistry

- Doctoral Thesis: *Improved Dynamics in Hybrid Particle-Field Simulations of Polymers*
- Advisor: **Prof. Dr. rer. nat. Florian Müller-Plathe**

The Univeristy of Akron *United States, Aug. 2016 - June 2018*
M.Sc. in Polymer Engineering

- Master Thesis: *Investigating the Effects of Grafting and Chain Stiffness on Nanoconfined Polymers from Molecular Dynamics Simulation*
- Advisor: **Prof. David S. Simmons**

Soochow University *China, Aug. 2013 - June 2016*
B.Sc. in Chemical Engineering

PEER-REVIEWED PUBLICATIONS

(**†equal contribution, ‡corresponding author**)

(16) **Wu, Z.**‡; Zhou, T. Structural Coarse-Graining via Multi-Objective Optimization with Differentiable Simulation *ChemRxiv* **2023**, preprint, DOI: 10.26434/chemrxiv-2023-177pg (under review)

(15) **Wu, Z.**; Zhou, T.‡; Lan, X.; Xu, C.; AI-Driven Innovative Design of Chemicals in Practice and Perspective, *Chemical Industry and Engineering Progress* **2023**, in publication, DOI: 10.16085/j.issn.1000-6613.2023-0811

(14) **Wu, Z.**; Pal, S.; Keten, S.‡; Implicit Chain Particle Model for Polymer Grafted Nanoparticles, **2023**, *Macromolecules* **2023** 56 (9), 3259-3271

(13) Fu. X.‡; **Wu, Z.**; Wang, W.; Xie, T.; Keten, S.; Gómez-bombarelli, R; Jaakkola, T.; Forces are not Enough: Benchmark and Critical Evaluation for Machine Learning Force Fields with Molecular Simulations, *TMLR*, **2022**, Preprint: https://arxiv.org/pdf/2210.07237v1.pdf

(12) Wang, W.†; **Wu, Z.**†; Gómez-Bombarelli, R.‡ Learning Pair Potentials using Differentiable Simulations, *J. Chem. Phys.* **2022**, 158 (4), Preprint: https://arxiv.org/pdf/2209.07679.pdf

(11) **Wu, Z.**; Müller-Plathe, F.‡; Hybrid Particle-Field Model with Slip-Springs for Coarse-Graining Branched Polymer Melts: Polystyrene Melts as An Example *J. Chem. Theory Comput.* **2022** 18 (6), 3814-3828

(10) **Wu, Z.**; Milano, G.; Müller-Plathe, F.‡ Combination of Hybrid Particle-Field Molecular Dynamics and Slip-Springs for the Efficient Simulation of Coarse-Grained Polymer Models: Static and Dynamic Properties of Polystyrene Melts *J. Chem. Theory Comput.* **2021**, 17 (1), 474-487

(9) **Wu, Z.**; Kalogirou, A.; De Nicola, A.; Milano, G.; Müller-Plathe, F.‡; Atomistic Hybrid Particle-

field Molecular Dynamics Combined with: Restoring Entangled Dynamics to Simulations of Polymer Melts *J. Comput. Chem.* **2021**, 42 (1), 6–18.

(8) Zhou, T.[†]; **Wu, Z.**[†‡]; Chilukoti, H. K.; Müller-Plathe, F.; Sequence-Engineering Polyethylene Polypropylene Copolymers with High Thermal Conductivity Using a Molecular-Dynamics-Based Genetic Algorithm *J. Chem. Theory Comput.* **2021**, 17 (6), 3772–3782.

(7) **Wu, Z.**[†]; Alberti, S. A. N.[†]; Schneider, J.; Müller-Plathe, F.[‡]; Knotting Behaviour of Polymer Chains in the Melt State for Soft-Core Models with and without Slip-Springs. *J. Phys.: Condens. Matter* **2021**, 33 (24) , 244001.

(6) Zhou, T.; **Wu, Z.**; Das, S.; Eslami, H.[‡]; Müller-Plathe, F. How Ethanolic Disinfectants Disintegrate Coronavirus Model Membranes: A Dissipative Particle Dynamics Simulation Study. *J. Chem. Theory Comput.* **2022**, 18 (4), 2597–2615.

(5) Zhou, T.; **Wu, Z.**; Das, S.; Eslami, H.[‡]; Müller-Plathe, F. Compatibilization Efficiency of Graft Copolymers in Incompatible Polymer Blends: Dissipative Particle Dynamics Simulations Combined with Machine Learning. *Macromolecules* **2022**, 55 (17), 7893-7907

(4) Zhan, Y.[†]; Li, W.[†]; Jiang, T.,; Fasel, C.; Ricohermoso, E.; Bernauer, J.; Yu Z.[‡]; **Wu, Z.**[‡]; Müller-Plathe, F.; Molina-Luna, L.; Grottenmüller, R.; Riedel, R.; Boron-Modified Perhydropolysilazane towards Facile Synthesis of Amorphous SiBN Ceramic with Excellent Thermal Stability. *J. Adv. Ceram.* **2022** 11, 1104–1116.

(3) Das, S.[‡]; Meinel, M. K.; **Wu, Z.**; Müller-Plathe, F. The Role of the Envelope Protein in the Stability of a Coronavirus Model Membrane against an Ethanolic Disinfectant. *J. Chem. Phys.* **2021**, 154 (24), 245101.

(2) Zhou, T.; Schneider, J.; **Wu, Z.**; Müller-Plathe, F.[‡] Compatibilization Efficiency of Additives in Homopolymer Blends: A Dissipative Particle Dynamics Study. *Macromolecules* **2021**, 54 (20), 9551–9564.

(1) Zhou, T.[†‡]; Chilukoti, H. K.[†‡]; **Wu, Z.**; Müller-Plathe, F. Effect of Defects on the Interfacial Thermal Conductance between N-Heneicosane in Solid and Liquid Phases and a Graphene Monolayer. J. *Phys. Chem. C* **2021**, 125 (25), 14149–14162.

FUNDINGS / PROJECTS

[2] Improving Polymer Upcycling via Sequence Engineering of Copolymer Compatibilizer, XJTLU Research Development Funding, Principle Investigator, Jan. 2024 - Dec. 2026

[1] Integrated Software Development for Molecular Modeling of Crude Oil, State Key Laboratory of Heavy Oil Open Project, Principle Investigator, Sep. 2023 - Aug. 2025

TEACHING / MENTORING EXPERIENCE

Undergraduate Teaching Assistant

Technische Universität Darmstadt — *Mar. 2019 - July 2019*
Physical Chemistry I Led group tutorial per week

Technische Universität Darmstadt — *Oct. 2020 - Feb. 2021*
Physical Chemistry II Led group tutorial per week

Technische Universität Darmstadt — *Mar. 2020 - July 2020*
Physical Chemistry III Led group tutorial per week

Graduate Teaching Assistant

Technische Universität Darmstadt — *Oct. 2019 - Feb. 2020*
Solid State Physics Prepared exercises and led group tutorial per week

Undergraduate Mentorship

Northwestern University *June 2022 - 2023*

- Mentoring an undergraduate student: Gave orientation and training on molecular dynamics simulations; We are investigating mechanical properties of matrix-free polymer grafted nanoparticles using multiscale molecular simulations.

Graduate Mentorship

Technische Universität Darmstadt *Apr. 2019 - July 2019*

- Mentoring a Master student during his praktikum(internship): Gave orientation and training on molecular dynamics simulations; Ideation and realization of the research project to investigate structural and dynamical properties of star-shaped polymer melts using coarse-grained molecular dynamics simulations.

PRESENTATIONS/ POSTERS

[Talk] Implicit Chain Particle Model for Polymer-Grafted Nanoparticles, APS Las Vegas, March 2023

[Talk] hPF-MD.jl: Hybrid Particle-Field Molecular Dynamics Simulation, JuliaCon2021, online, July 2021

[Talk] Sequence Engineering Thermal conductivity of Copolymers using Molecular-Dynamics-Based Genetic Algorithm, Soochow University, Online, May 2021

[Talk] Atomistic Hybrid Particle-Field Molecular Dynamics Combined with Slip-Springs: Restoring Entangled Dynamics to Simulations of Polymer Melts, CECAM/IRTG school: Bio/Soft Matter Simulations across Multiple Scales, Heidelberg Germany, Sep. 2019

[Poster] Systematic Coarse-Graining of Polymers through Automatic Differentiation, CECAM workshop: Recent Advances in Machine Learning Accelerated Molecular Dynamics, Online, Mar. 2022

[Poster] Combination of Slip-Springs with Hybrid-Particle-Field Molecular-Dynamics for Polymer Dynamics, Mainz Materials Simulations Days 2019, Mainz, June 2019

[Poster] Multi-chain Slip-spring Hybrid Particle-field Model for Molten Polyethylene, Bunsentagung 2019, Jena, May 2019

REVIEW SERVICE

Macromolecules (2);
npj Computational Materials (1);
Soft Matter (1);
Journal of Engineering Mechanics (1).

LANGUAGES

English, Chinese (Mandarin, Wu), German