Zhenghao Wu

CONTACT INFORMATION

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RESEARCH INTERESTS

Chemical Theory and Computation; Computational Materials Science and Mechanics; Interpretable Machine Learning; Statistical Mechanics

EMPLOYMENT

Northwestern University *United States, Nov. 2021 - Present*
Department of Civil and Environmental Engineering

- Topic: *Multiscale Simulations of Polymers and Their Nanocomposites*
- 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

Deeplearning.ai *Coursera*
Deep learning courses: Improving Deep Neural Networks, Hyperparameter Tuning, Regularization and Optimization; Structuring Machine Learning Projects

PREPRINT / SUBMITTED

(†**equal contribution,** ‡**corresponding author**, 3 in total with 2 first-authored)
(3) **Wu, Z.**; Pal, S.; Keten, S.‡; Implicit Chain Particle Model for Polymer Grafted Nanoparticles, **2022**, Submitted to *Macromolecules*, Preprint available upon request.

(2) 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, **2022**, Submitted to *ICLR*, Preprint: https://arxiv.org/pdf/2210.07237v1.pdf

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

PEER-REVIEWED PUBLICATIONS

(†**equal contribution,** ‡**corresponding author**, 11 in total with 5 first-authored)
(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.

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 - Present*

- 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] 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