

# Zhengkao Wu

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RESEARCH INTERESTS	<i>Chemical Theory and Computation; Computational Materials Science and Mechanics; Interpretable Machine Learning; Statistical Mechanics</i>	
EMPLOYMENT	<b>Northwestern University</b> Department of Civil and Environmental Engineering <ul style="list-style-type: none"><li>• Topic: <i>Multiscale Simulations of Polymers and Their Nanocomposites</i></li><li>• Advisor: <b>Prof. Sinan Keten</b></li></ul>	<i>United States, Nov. 2021 - Present</i>
EDUCATION	<b>Technische Universität Darmstadt</b> Dr. rer. nat. in Theoretical Chemistry <ul style="list-style-type: none"><li>• Doctoral Thesis: <i>Improved Dynamics in Hybrid Particle-Field Simulations of Polymers</i></li><li>• Advisor: <b>Prof. Dr. rer. nat. Florian Müller-Plathe</b></li></ul>	<i>Germany, Aug. 2018 - Oct. 2021</i>
	<b>The University of Akron</b> M.Sc. in Polymer Engineering <ul style="list-style-type: none"><li>• Master Thesis: <i>Investigating the Effects of Grafting and Chain Stiffness on Nanoconfined Polymers from Molecular Dynamics Simulation</i></li><li>• Advisor: <b>Prof. David S. Simmons</b></li></ul>	<i>United States, Aug. 2016 - June 2018</i>
	<b>Soochow University</b> B.Sc. in Chemical Engineering	<i>China, Aug. 2013 - June 2016</i>
	<b>DeepLearning.ai</b> Deep learning courses: Improving Deep Neural Networks, Hyperparameter Tuning, Regularization and Optimization; Structuring Machine Learning Projects	<i>Coursera</i>
PREPRINT / SUBMITTED	<b>(<sup>†</sup>equal contribution, <sup>‡</sup>corresponding author)</b> (3) <b>Wu, Z.</b> ; Pal, S.; Keten, S. <sup>‡</sup> ; Implicit Chain Particle Model for Polymer Grafted Nanoparticles, <b>2022</b> , Submitted to <i>Macromolecules</i> , Preprint available upon request.  (2) Fu, X. <sup>‡</sup> ; <b>Wu, Z.</b> ; 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, <b>2022</b> , Submitted, Preprint: <a href="https://arxiv.org/pdf/2210.07237v1.pdf">https://arxiv.org/pdf/2210.07237v1.pdf</a>  (1) Wang, W. <sup>†</sup> ; <b>Wu, Z.</b> <sup>†</sup> ; Gómez-Bombarelli, R. <sup>‡</sup> Learning Pair Potentials using Differentiable Simulations, <b>2022</b> , Accepted, <i>J. Chem. Phys.</i> , Preprint: <a href="https://arxiv.org/pdf/2209.07679.pdf">https://arxiv.org/pdf/2209.07679.pdf</a>	
PEER-REVIEWED PUBLICATIONS	<b>(<sup>†</sup>equal contribution, <sup>‡</sup>corresponding author)</b> (11) <b>Wu, Z.</b> ; Müller-Plathe, F. <sup>‡</sup> ; Hybrid Particle-Field Model with Slip-Springs for Coarse-Graining Branched Polymer Melts: Polystyrene Melts as An Example <i>J. Chem. Theory Comput.</i> <b>2022</b> 18 (6), 3814-3828  (10) <b>Wu, Z.</b> ; Milano, G.; Müller-Plathe, F. <sup>‡</sup> 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 <i>J. Chem. Theory Comput.</i> <b>2021</b> , 17 (1), 474-487  (9) <b>Wu, Z.</b> ; Kalogirou, A.; De Nicola, A.; Milano, G.; Müller-Plathe, F. <sup>‡</sup> ; Atomistic Hybrid Particle-field Molecular Dynamics Combined with: Restoring Entangled Dynamics to Simulations of Poly-	

mer Melts *J. Comput. Chem.* **2021**, 42 (1), 6–18.

(8) Zhou, T.<sup>†</sup>; **Wu, Z.**<sup>†‡</sup>; 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.**<sup>†</sup>; Alberti, S. A. N.<sup>†</sup>; Schneider, J.; Müller-Plathe, F.<sup>‡</sup>; 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.<sup>‡</sup>; 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.<sup>‡</sup>; 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.<sup>†</sup>; Li, W.<sup>†</sup>; Jiang, T.; Fasel, C.; Ricohermoso, E.; Bernauer, J.; Yu Z.<sup>‡</sup>; **Wu, Z.**<sup>‡</sup>; 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.<sup>‡</sup>; 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.<sup>‡</sup> Compatibilization Efficiency of Additives in Homopolymer Blends: A Dissipative Particle Dynamics Study. *Macromolecules* **2021**, 54 (20), 9551–9564.

(1) Zhou, T.<sup>†‡</sup>; Chilukoti, H. K.<sup>†‡</sup>; **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