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ACADEMIC EXPERIENCE:

- (1). 2001.9-2005.7: Undergraduate student, Department of Chemistry, Jilin University;
- (2). 2005.9-2010.7: Ph. D student, Institute of Theoretical Chemistry, Jilin University;
- (3). 2010.7-2012.9: Lecture, State Key Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University;
- (4). 2012.9-2018.12: Associate professor, State Key Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University.

During which: 2015.5-2016.8: Humboldt fellow, Technical University of Darmstadt (Germany). In cooperation with Prof. Florian Müller-Plathe.

(5) 2018.12-present: Professor, Key Laboratory of Theoretical Chemistry of Environment Ministry of Education, School of Environment, South China Normal University.

AWARDS:

- (1). Winner of Hong Kong “Qiu Shi” Postgraduate Award (2008);
- (2). Winner of the first “Foundation for Distinguished Young Scholars”, College of Chemistry, Jilin University (2009);
- (3). Outstanding award of the 24th “Elite Cup” Academic Achievement Contest, Jilin University (2009);
- (4). Fellowship of Alexander von Humboldt Foundation, Germany (2015);
- (5). Excellent reviewer of the Chinese Journal of Polymer Science (2023).

FUNDING SUPPORT:

- 1) National Science Fund for Excellent Young Scholars of China (优青) (22022303)
- 2) National Science Foundation of China (21104025;21474042; 21774051)
- 3) China Postdoctoral Science Foundation (20110491295)
- 4) China Postdoctoral Science Foundation: Special Support (2012T50286)

SCIENTIFIC INTRODUCTION:

Dr. Hong Liu obtained his bachelor’s and doctoral degree in Jilin University at 2005 and 2010, respectively. His research interest focuses on the mesoscopic behavior of the reactive polymer systems, as well as the topological regulations of mechanical interlocked polymers. Dr. Liu had developed a coarse-grained simulation strategy coupled with the polymerization reaction model, which had been applied by others including international renowned scholars for many times. His work has established the multi-scale theoretical and simulation study framework of the structure and dynamics of macromolecular systems mediated by microscopic

molecular reactions. Till now, more than 100 peer-reviewed papers have been published on the journals like *Science*, *Macromolecules*, etc.

SELECTED PUBLICATIONS:

1. Wang, Y.; Lu, H.; Jia, X.-M.; Shi, A.-C.*; Zhou, J.*; Zhang, G.*; **Liu, H.***, Entropy-Induced Localization and Sliding Dynamics of Rings on Polyrotaxane. *Macromolecules* **2024**, *57*(4), 1846-1858.
2. Zhang, Z.; Zhao, W.; Cheng, Z.; Zhang, G.*; **Liu, H.***, Olympic Gels Formed through Catenation of DNA Rings Regulated by Topoisomerase II: A Coarse-Grained Model. *The Journal of Chemical Physics* **2024**, *160*(5), 054906.
3. Mao, J.; Zhou, J.*; **Liu, H.***, One-pot strategy for the preparation of nanoparticles grafted with bimodal polymers: An in-silico insight. *Composites Science and Technology* **2024**, *251*, 110583.
4. Liu, W.; Zhang, J.*; **Liu, H.***, Morphology evolution and dynamics of sliding nanodroplets under external forces: A molecular dynamics study. *Physics of Fluids* **2023**, *35* (8), 082010.
5. Wang, Y.; Gan, H.-L.; Liang, C.-X.; Zhang, Z.-Y.; Xie, M.; Xing, J.-Y.; Xue, Y.-H.; **Liu, H.***, Network structure and properties of crosslinked bio-based epoxy resin composite: An in-silico multiscale strategy with dynamic curing reaction process. *Giant* **2021**, *7*, 100063.
6. **Liu, H.**; Xue, Y.-H.; Zhu, Y.-L.; Gu, F.-L.; Lu, Z.-Y.*, Inverse Design of Molecular Weight Distribution in Controlled Polymerization via a One-Pot Reaction Strategy. *Macromolecules* **2020**, *53* (15), 6409-6419.
7. Yi, C.; **Liu, H.**; Zhang, S.; Yang, Y.; Zhang, Y.; Lu, Z.; Kumacheva, E.*; Nie, Z.*, Self-limiting directional nanoparticle bonding governed by reaction stoichiometry. *Science* **2020**, *369* (6509), 1369-1374.
8. Yan, Y.-D.; Xue, Y.-H.; Zhao, H.-Y.; **Liu, H.***; Lu, Z.-Y.; Gu, F.-L., Insight into the Polymerization-Induced Self-Assembly via a Realistic Computer Simulation Strategy. *Macromolecules* **2019**, *52* (16), 6169-6180.
9. Xing, J.-Y.; Xue, Y.-H.; Lu, Z.-Y.*; **Liu, H.***, In-Depth Analysis of Supramolecular Interfacial Polymerization via a Computer Simulation Strategy. *Macromolecules* **2019**, *52*

- (17), 6393-6404.
10. **Liu, H.**; Zhao, H.-Y.; Müller-Plathe, F.; Qian, H.-J.; Sun, Z.-Y.; Lu, Z.-Y.*, Distribution of the Number of Polymer Chains Grafted on Nanoparticles Fabricated by Grafting-to and Grafting-from Procedures. *Macromolecules* **2018**, *51* (10), 3758-3766.
 11. Xue, Y.-H.; Quan, W.; Liu, X.-L.; Han, C.; Li, H.; **Liu, H.***, Dependence of Grafted Polymer Property on the Initiator Site Distribution in Surface-Initiated Polymerization: A Computer Simulation Study. *Macromolecules* **2017**, *50* (17), 6482-6488.
 12. **Liu, H.***; Zhu, Y.-L.; Lu, Z.-Y.; Müller-Plathe, F., A kinetic chain growth algorithm in coarse-grained simulations. *Journal of Computational Chemistry* **2016**, *37* (30), 2634-2646.
 13. **Liu, H.**; Zhu, Y. L.; Zhang, J.; Lu, Z. Y.*; Sun, Z. Y.*, Influence of Grafting Surface Curvature on Chain Polydispersity and Molecular Weight in Concave Surface-Initiated Polymerization. *ACS Macro Letters* **2012**, *1* (11), 1249-1253.
 14. **Liu, H.**; Li, M.*; Lu, Z. Y.*; Zhang, Z. G.; Sun, C. C.; Cui, T., Multiscale Simulation Study on the Curing Reaction and the Network Structure in a Typical Epoxy System. *Macromolecules* **2011**, *44* (21), 8650-8660.
 15. **Liu, H.**; Li, M.; Lu, Z. Y.*; Zhang, Z. G.; Sun, C. C., Influence of Surface-Initiated Polymerization Rate and Initiator Density on the Properties of Polymer Brushes. *Macromolecules* **2009**, *42* (7), 2863-2872.