Qilu Yuan

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Education Background

Sept 2021-Now **University of Science and Technology of China**, Hefei, Anhui, China
Major: Chemistry, Doctor of Philosophy

Sept 2021-Now **Changchun Institute of Applied Chemistry**, Changchun, Jilin, China
Major: Chemistry, Doctor of Philosophy

Aug 2017-Jun 2021 **Ocean University of China**, Qingdao, Shandong, China
Major: Polymer Materials and Engineering, Bachelor of Engineering

Research Experience

Feb 2022-Now **Dynamics of Amorphous Polymer**
Simulation of glass formation of polymeric systems via LAMMPS, especially glass formation of polymer-additive composite;

Oct 2018-May 2020 **Application of High-Temperature Resistant Cerium-based Materials in Various Catalytic Oxidation Reactions**
Investigation of the catalytic performance of a series of nanostructured Ag/CeO_2 materials in practical applications ;

Publications

1) **Q.-L. Yuan**; X. Xu; J. F. Douglas*; W.-S. Xu*, Physical Origin of the Mass Dependence of Glass Transition Temperature and Fragility of Polymer Liquids, *Macromolecules*, **2025**, 58(17), 9528 9545.

2) **Q.-L. Yuan**; X. Xu; J. F. Douglas*; W.-S. Xu*, Understanding Relaxation in the Kob-Andersen Liquid Based on Entropy, String, Shoving, Localization, and Parabolic Models, *J. Phys. Chem. B*, **2024**, 128(40), 10999-11021.

3) **Q.-L. Yuan**; X. Xu; J. F. Douglas*; W.-S. Xu*, Influence of Density and Pressure on Glass Formation in the Kob–Andersen Model, *J. Phys. Chem. B*, **2024**, 128(40), 9889-9904.

4) **Q.-L. Yuan**; Z. Yang; W.-S. Xu*, Advances in the generalized entropy theory of polymer glass formation, *Sci. Sin. Chim.*, **2023**, 53(4), 616-627.

5) Y. Cao; **Q.-L. Yuan**; Q. Chen; W.-S. Xu*, Influence of Charge Interaction Strength and Counterion Size on the Structure and Dynamics of Simulated Telechelic Ionomer Melts, *Macromolecules*, **2025**, 58(6), 2829-2849.

6) J. F. Douglas*; **Q.-L. Yuan**; J. Zhang; H. Zhang*; W.-S. Xu*, A dynamical system approach to relaxation in glass-forming liquids, *Soft Matter*, **2024**, 20(46), 9140-9160.

7) X.Y. Song; Z. Yang; **Q.-L. Yuan**; S. Li; Z.-Q. Tang; Y.-T. Dong; S. Jiang*; W.-S. Xu*; et al. Understanding Mass Dependence of Glass Formation in Ring Polymers, *Chin. J. Polym. Sci.*, **2023**, in press

Skills

Proficient in Polymer Physics, Polymer Glass Formation
Proficient in Lammps, Gromacs, Python, Fortran, C++, LaTeX
Knowledge and experience in Linux, Bash Shell, Git, CMake