Yiling Nan

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Website, Google Scholar

SUMMARY STATEMENT

- Research expertise in computational simulation (molecular modeling and parameter optimization) and experimental polymer chemistry & physics (polymer design, synthesis, and analysis).
- Strong publication record with 9 first-author (1 under review) articles and a total of 21 publications in prestigious journals, including *Science, Angew., Chem J. Chem. Theory Comput*., etc.
- Strong programming skills demonstrated by the development of custom in-house programs for parameter optimization and data analysis.
- Demonstrated leadership and collaboration skills, highlighted through co-authored publications and mentoring experience.

EMPLOYMENT

Postdoc Research Fellow in School of Pharmacy — Aug. 2022 – Present
University of Maryland Baltimore, Baltimore, US

EDUCATION

Ph.D. in Civil and Environmental Engineering — Jun. 2022
Petroleum Engineering (*GPA:3.95/4.00*)
University of Alberta, Edmonton, Canada

Master in Chemistry and Biotechnology — Aug. 2018
The University of Tokyo, Tokyo, Japan

Bachelor in Chemical Engineering — Jul. 2016
Tsinghua University, Beijing, China

SKILLS

- Computer skills: C, Python, BASH, MATLAB, ASPEN, AutoCAD, OPENMM, CHARMM, GROMACS, NAMD, VMD, PSI4, Gaussian
- Experimental skills: NMR, DSC, TGA, FT-IR, UV-Vis, LS (Light Scattering), GPC, DMA, SEM, TEM, Rheometer, etc.
- Language skills: English (Fluent), Mandarin (Native), Korean (Native), Japanese (Fluent).

SELECTED RESEARCH EXPERIENCE

ForceField (FF) Parameter Optimization and Development

2022 - Present

- Led a world-class team in parameter optimization, contributing to collaborative publications under preparation.
- Developed a software tool in BASH and Python to automate FF parameter generation based on potential energy scans, enabling continuous FF optimization.
- 3 conference presentations with 1 paper published on "*J. Chem. Theory Comput.*" and 2 under preparation.
- Improved the forcefield performance in producing thermodynamic properties by up to 50 % with the new set of parameters.

Fluid Distribution and Transport in Nano-Confined Space

2016, 2018 - 2022

- Conducted molecular dynamics simulations to analyze the flow characteristics of both compressible and incompressible fluids within nano porous media.
- Developed in-house C codes to quantify the fluid flux deviation from the Navier-Stokes (N-S)

equation using a user-friendly parameter (slip length) for numerical simulation.
- Published 6 peer-reviewed full-length articles (2 as the first author).
- Delivered comprehensive insights into slip length, enhancing the understanding of fluid transport in nanoscale media with broad applications in nanotechnology.

Multiphase Interfacial Properties involved Surface-Active Agents (Colloids)

2018 - 2022

- Simulated the distribution and roles of surface-active agents at the multiphase interfaces (liquid-liquid, liquid-gas, liquid-solid) using the molecular dynamics simulation.
- Developed the in-house C and MATLAB codes to analyze the configurational (atomic scale) and thermodynamics (macro-scale) properties.
- Published 8 peer-reviewed full-length articles or a book chapter (5 as the first author).
- Established a robust theoretical framework essential for designing surfactant formulations applicable to real-world industrial challenges.

Sustainable Self-Healable Polymer Glass (Polymer Physics)

2016 - 2018

- Polymer synthesis and polymer blend preparation.
- Characterization of the polymer using NMR (solution, and solid-state), MALS, GPC, IR, Rheology, TGA, and DSC, etc.
- Increased Yong's modulus by 50 times compared to existing intrinsic self-healing materials. Promising material with far-reaching applications in cabin windows and electric products screens etc. with extended lifetime.
- Published 2 peer-reviewed papers in "*Science*", and "*Angew. Chem*".

AWARDS

- Donald Lougheed Engineering Graduate Scholarship (~ 5/1600, ~ 4400 USD), University of Alberta — 2021
- Doctoral Recruitment Scholarship (~ 7400 USD), University of Alberta — 2018
- Nagashima Scholarship (4/3800, ~ 360 USD / month), The University of Tokyo — 2017-2018
- SK Group Scholarship (~1400 USD / year), Tsinghua University — 2012-2016

SELECTED PUBLICATIONS (4/21) and PRESENTATIONS (2/14)

- **Y. Nan**, A. MacKerell, Balancing Group I Monatomic Ion–Polar Compound Interactions for Condensed Phase Simulation in the Polarizable Drude Force Field, *J. Chem. Theory Comput.,* **2024***, 20, 8, 3242–3257*
- **Y. Nan**, W. Li, Z. Jin, Slip length of methane flow under shale reservoir conditions: Effect of pore size and pressure, *Fuel*, **2020**, *259*: 116237
- **Y. Nan**, W. Li, M. Zhang, Z. Jin, Ethanol Blending to Improve Reverse-Micelle Dispersity in Supercritical CO2: A Molecular Dynamics Study, *J. Phys. Chem. B,* **2021***, 125 (33)*: 9610-9620
- Y. Yanagisawa, **Y. Nan**, K. Okuro, T. Aida, Mechanically robust, readily repairable polymers via tailored noncovalent cross-linking*. Science,* **2018**, *359(6371)*: 72 – 76.
- **Y. Nan,** A. MacKerell; " Balancing Monoatomic Ion-Biomolecular Interactions in the Polarizable Drude Force Field", ACS Spring, Mar. 27, 2023. (oral)
- **Y. Nan,** Z. Jin; " Understanding the Role of Surface-Active Chemical Additives in Enhanced Oil Recovery from Molecular Perspectives", Student Seminar Series (3S) in ACS, Dec. 10, 2021. (oral presentation) ***Invited Talk ****

LEADESHIP & SERVICE

- **Journal Reviews:** Chemical Engineering Journal; Langmuir; Fuel; Journal of Molecular Liquids Colloids and Surfaces A: Physicochemical and Engineering Aspects *etc*.
- **Research Mentoring:** Mentored five Master's and Ph.D. students, resulting in collaborative publications.