Yiling Nan

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EMPLOYMENT

Assistant Professor in Chemical and Petroleum Engineering
The University of Kansas, Lawrence, US — Aug. 2025 -

Postdoc Research Fellow in School of Pharmacy,
Center of Computer Aided Drug Design (CADD),
University of Maryland Baltimore, Baltimore, US — Aug. 2022 – Aug. 2025

EDUCATION

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

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

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

AWARDS

- ACCESS Allocation Request CHM250084 (~ 1000 USD) — 2025
- Contributions to Science, ACS ENFL
- 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

PEER-REVIEWED JOURNAL PUBLICATIONS

- **Y. Nan**, P. Baral, Orr A A, et al. Balancing Group 1 Monoatomic Ion–Polar Compound Interactions in the Polarizable Drude Force Field: Application in Protein and Nucleic Acid Systems. *J. Phys. Chem. B*, **2024**, 128(49): 12078-12091
- **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*
- W. Li, **Y. Nan**, Z. Jin, Dependence of Methane Transport on Pore Informatics in the Amorphous Nanoporous Kerogen Matrix, *Langmuir,* **2024**, 40, *1*, 687–695
- L. Duan, M. Zhang, **Y. Nan**, Z. Jin, Effects of Interfacial Molecular Structures on Pressure-Driven Brine Flow in Silica Mesopores, *Langmuir,* **2023**, 39, *37*, 13019–13027
- M. Zhang, **Y. Nan**, Y. Lu, Q. You, Z. Jin, CO2-responsive surfactant for oil-in-water emulsification and demulsification from molecular perspectives, *Fuel,* **2023***, 331 (2)*: 125773
- Y. Fujisawa, **Y. Nan**, A. Asano, Y. Yanagisawa, K. Yano, Y. Itoh, T. Aida, Blending to Make Nonhealable Polymers Healable: Nanophase Separation Observed by CP/MAS 13C NMR Analysis, *Angew. Chem. Int. Ed.*, **2022**, e202214444
- **Y. Nan**, Z. Jin, Effect of Alcohol Tail Length on Aggregate Behavior of Alcohol and AOT at the Water-scCO2 Interface: MD Simulation Study, Book, *Nanostructured Materials for Sustainable*

Energy: Design, Evaluation, and Applications, Chapter 10, pp 263-288, **2022**

- **Y. Nan**, W. Li, Z. Jin, Molecular Dynamics Studied on Effective Surface-Active Additives: Toward Hard Water-Resistant Chemical Flooding for Enhanced Oil Recovery, *Langmuir,* **2022***, 38 (16)*: 4802-4811
- **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. Nan**, W. Li, Z. Jin, Ion Valency and Concentration Effect on the Structural and Thermodynamic Properties of Brine-Oil Interfaces with Anionic Surfactant (SDS), *J. Phys. Chem. B,* **2021***, 125 (33)*: 9621-9628
- X. Zhang*, Q. Jin*, **Y. Nan***, L. Hou, B. Li, X. Chen, Z. Jin, X. Zhang, J. Huang, and Q. Zhang, Electrolyte Structure of Lithium Polysulfides with Anti-Reductive Solvent Shells for Practical Lithium-Sulfur Batteries, *Angew. Chem. Int. Ed.*, **2021**, *60*: 15503-15509 **Co-first Author*
- W. Li, **Y. Nan**, Q. You, Z. Jin, CO2 solubility in brine in silica nanopores in relation to geological CO2 sequestration in tight formations: Effect of salinity and pH, *Chem. Eng. J.*, **2021**, *411:* 127626
- W. Li, M. Zhang, **Y. Nan,** W. Pang, Z. Jin, Molecular Dynamics Study on CO2 Storage in Water-Filled Kerogen Nanopores in Shale Reservoirs: Effects of Kerogen Maturity and Pore Size, *Langmuir.*, **2021**, *37(1):* 542–552
- W. Li, **Y. Nan**, Z. Zhang, Q. You, Z. Jin, Hydrophilicity/Hydrophobicity Driven CO2 Solubility in Kaolinite Nanopores in Relation to Carbon Sequestration, *Chem. Eng. J.*, **2020**, *398:* 125449
- **Y. Nan**, W. Li, Z. Jin, Roles of alcohol as a cosurfactant at brine-oil interface under a typical reservoir condition, *Langmuir*, **2020**, *36(19):* 5198-5207
- W. Li, **Y. Nan**, Q. You, Q. Xie, Z. Jin, Effects of salts and silica nanoparticles on oil-brine interfacial properties under hydrocarbon reservoir conditions: A molecular dynamics simulation study, *J. Mol. Liq.*, **2020**, *305*: 112860
- X. Hu, **Y. Nan**, X. Kong, D. Lu, and J. Wu, A hybrid theoretical method for predicting electrokinetic energy conversion in nanochannels, *Phys. Chem. Chem. Phys.*, **2020**, *22(16)*: 9110-9116
- **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
- W. Li, **Y. Nan**, X. Wen, W. Wang, Z. Jin, Effects of Salinity and N-, S-, and O-Bearing Polar Components on Light Oil–Brine Interfacial Properties from Molecular Perspectives, *J. Phys. Chem. C*, **2019**, 123, 38, 23520-23528
- 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**, X. Kong, J. Li, D. Lu, Non-equilibrium Molecular Dynamics Simulation of Water Flow Inside Nano-slit. *Journal of Chemical Industry and Engineering*, **2017**, *68(5)*: 1786 – 1793.

PRESENTATIONS

- **Y. Nan,** A. MacKerell; " Balancing Monoatomic Ion-Biomolecular Interactions in the Polarizable Drude Force Field", CADD Symposium, May. 25, 2023. (poster presentation)
- **Y. Nan,** A. MacKerell; " Balancing Monoatomic Ion-Biomolecular Interactions in the Polarizable Drude Force Field", CADD Symposium, Jul. 20, 2024. (poster presentation)
- **Y. Nan,** A. MacKerell; " Balancing monoatomic ion-biomolecular interactions in the polarizable Drude force field", Biophysical Society, Feb. 8, 2024. (poster presentation)
- **Y. Nan,** A. MacKerell; " Balancing Monoatomic Ion-Biomolecular Interactions in the Polarizable Drude Force Field", AIChE, Nov. 6, 2023. (poster presentation)

- **Y. Nan,** A. MacKerell; " Balancing Monoatomic Ion-Biomolecular Interactions in the Polarizable Drude Force Field", CADD Symposium, May. 25, 2023. (poster presentation)
- **Y. Nan,** A. MacKerell; " Balancing Monoatomic Ion-Biomolecular Interactions in the Polarizable

Drude Force Field", ACS Spring, Mar. 27, 2023. (oral presentation)

- **Y. Nan,** Z. Jin; " Interfacial Electrolyte Structure with Anti-Reductive Solvent at Electrode for Practical Lithium-Sulfur Batteries: A Molecular Dynamics Study", AIChE, Nov. 16, 2022. (oral presentation Z.Jin presented)
- **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 ****
- **Y. Nan,** Z. Jin; " Electrolyte Design in Li-S battery with anti-reductive solvent shell", Future energy systems 2021 research symposium. Sept. 20-24, 2021. (oral presentation)
- **Y. Nan,** Z. Jin; " Effect of salt ion valency and concentration on the structural and thermodynamic properties of SDS and propanol at brine-oil interfaces from molecular perspectives", ACS Fall 2021 Virtual Conference. Aug. 22-26, 2021. (oral presentation)
- **Y. Nan,** Z. Jin; " Why alcohols can improve reverse-micelle dispersity in supercritical CO2?: A molecular-level understanding", ACS Fall 2021 Virtual Conference. Aug. 22-26, 2021. (oral presentation)
- **Y. Nan,** Z. Jin; " Slip Length of Methane Flow under Shale Reservoir Conditions: Effect of Pore Size and Pressure", AIChE 2020 Virtual Conference. Nov. 16-20, 2020. (oral presentation)
- **Y. Nan,** Z. Jin; " Roles of Alcohol as a Cosurfactant at Brine-Oil Interface Under a Typical Reservoir Condition", AIChE 2020 Virtual Conference. Nov. 16-20, 2020. (oral presentation)
- **Y. Nan,** T. Aida; " Preparation of densely hydrogen-bonded polymer blends and their healing properties", 67th SPSJ Annual. May. 2018. (poster presentation)

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 more than five Master's and Ph.D. students, resulting in collaborative publications.