Tianmu Yuan

Postdoctoral Research Associate, School of Natural and Environmental Sciences, Newcastle University

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Research Interest

Statistical mechanics | Molecular Dynamics | Monte Carlo | Mean Field Theory | Density Functional Theory
Membrane Separation | Carbon Capture | Adsorption | Polymer | Energy | Battery

Education

PhD in Chemical Engineering Oct 2020 – Sept 2024
Department of Chemical Engineering, University of Manchester, UK

MSc in Advanced Chemical Engineering Sept 2016 – Nov 2017
Department of Chemical Engineering, Imperial College London, UK

BEng Hons. in Chemical Engineering with Year Long Work Placement Sept 2012 – Jun 2016
Department of Chemical Engineering, University of Bath, UK

Professional Experience

Postdoctoral Research Associate Dec 2024 –
School of Natural and Environmental Sciences, Newcastle University, UK

Research Assistant Sept 2024 – Nov 2024
Department of Chemical Engineering, University of Manchester, UK

Research Assistant Jan 2018 – Dec 2019
Department of Chemical and Biomolecular Engineering, Clemson University, US

Special Research Student Jun 2017 – Sept 2017
Graduate School of Frontier Sciences, University of Tokyo, Japan

Development Technician Jul 2014 – Jul 2015
Research and Development, Freudenberg Performance Materials, UK

Honors and Awards

Session Chair | Modelling and Simulation in Membrane Science | Euromembrane 2024 2024
Researcher Development and Travel Grant | Royal Society of Chemistry 2024
Chinese Government Award for Outstanding Self-financed Students Abroad | China Scholarship Council 2023
World Association of Membrane Societies Award: Oral Presentation | 13th International Congress on Membranes and Membrane Processes 2023
Researcher Development and Travel Grant | Royal Society of Chemistry 2023
Researcher Development Grants | Royal Society of Chemistry 2022
Overseas Research Scholar Award | 4-Year PhD Scholarship | The University of Manchester 2021
Graduate Teaching Assistant Award | The University of Manchester 2021

Teaching

Graduate Teaching Assistant, University of Manchester, UK Oct 2020 – Sept 2024

Graduate Level	Advanced Gas Separations | Chemical Engineering Molecular Simulations | Research Techniques and Methods | Reaction System Design
Undergrad Level	Batch Processing | Catalytic Reactor Engineering | Chemical Engineering Optimisation | Process Control | Process Design

Graduate Teaching Assistant, Clemson University, US Aug 2018 – Jan 2019

Undergrad Level	Thermodynamics II

PUBLICATIONS

*Corresponding Author,†Equal Contribution

6. ***Yuan, T.**, Giro, R., Steiner, M. B., Hsu. H., and Sarkisov, L., "Emergence of the Robeson bound in non-equilibrium molecular dynamics simulations", ***In preparation*** (2024).
5. ***Yuan, T.**, and Sarkisov, L., "How 2D nanoflakes improve transport in mixed matrix membranes: insights from a simple lattice model and dynamic mean field theory" ***ACS Appl. Mater. Interfaces***, 16.6 (2024): 8184-8195.
4. ***Yuan, T.**, De Angelis, M. G., and Sarkisov, L. "Simple lattice model explains equilibrium separation phenomena in glassy polymers. "***J. Chem. Phys.***, 159.5 (2023).
3. **Yuan, T.**, DeFever, R. S., Zhou, J., Cortes-Morales, E. C., *Sarupria, S., "RSeeds: Rigid seeding method for studying heterogeneous crystal nucleation." ***J. Phys. Chem. B.*** 127.18 (2023): 4112-4125.
2. ***Yuan, T.**, and Sarkisov L. "Lattice Model of Fluid Transport in Mixed Matrix Membranes." ***Adv. Theory Simul.***, 5.9 (2022): 2200159.
1. **Yuan, T.**, Farmahini, A. H. and *Sarkisov, L., "Application of Dynamic Lattice Mean Field Theory to fluid transport in slit pores." ***J. Chem. Phys.***, 155 (2021):074702.

PRESENTATION

Oral Talks

3. "Gas separation through polymer membranes: from both Equilibrium and NonEquilibrium Molecular Simulations", *Euromembrane2024*, Prague, Czechia, Sept, 2024
2. "Equilibrium separation phenomena in a simple lattice model of polymer membrane", *13th International Congress on Membranes and Membrane Processes*, Chiba, Japan, July, 2023 (**Oral Presentation Award**)
1. "Lattice Model of Fluid Transport in Mixed Matrix Membranes", *The 27th Thermodynamics Conference*, Bath, UK, Sept, 2022

Posters

3. "How 2D nanoflakes improve transport in mixed matrix membranes: insights from a simple lattice model and Dynamic Mean Field Theory", *13th International Congress on Membranes and Membrane Processes*, Chiba, Japan, July, 2023
2. "Application of dynamic mean field theory to study fluid transport in membranes" *The 14th International Conference on Fundamentals of Adsorption*, Denver, CO, US, May, 2022
1. "Rigid Seeding: A Computationally Efficient Method to Study Heterogeneous Nucleation in Molecular Simulations" *Crystal Growth and Assembly Gordon Research Conference*, Manchester, NH, US, June, 2019

PROFESSIONAL AFFILIATION

MRSC	Member | Royal Society of Chemistry (RSC)	2021-
AMIChemE	Associate Member | Institution of Chemical Engineers (IChemE)	2024-
AFHEA	Associate Fellow | Advance HE (formerly the Higher Education Academy)	2024-
Instructor	Snowboard Level 1 | British Association of Snowsport Instructors (BASI)	2024-

SKILLS

Programming	Python | C++ | C | Fortran | Bash | Tcl | LaTeX | CUDA
Web	HTML | CSS | JavaScript
OS	Linux/Unix | Mac | Windows
Safety	First Aid