

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 Department of Chemical Engineering, University of Manchester, UK	Oct 2020 – Sept 2024
MSc in Advanced Chemical Engineering Department of Chemical Engineering, Imperial College London, UK	Sept 2016 – Nov 2017
BEng Hons. in Chemical Engineering with Year Long Work Placement Department of Chemical Engineering, University of Bath, UK	Sept 2012 – Jun 2016

PROFESSIONAL EXPERIENCE

Postdoctoral Research Associate School of Natural and Environmental Sciences, Newcastle University, UK	Dec 2024 –
Research Assistant Department of Chemical Engineering, University of Manchester, UK	Sept 2024 – Nov 2024
Research Assistant Department of Chemical and Biomolecular Engineering, Clemson University, US	Jan 2018 – Dec 2019
Special Research Student Graduate School of Frontier Sciences, University of Tokyo, Japan	Jun 2017 – Sept 2017
Development Technician Research and Development, Freudenberg Performance Materials, UK	Jul 2014 – Jul 2015

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", *ChemRxiv* (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

AFFILIATION

Member	MRSC Royal Society of Chemistry (RSC)	2021-
Associate Member	AMIChemE Institution of Chemical Engineers (IChemE)	2024-
Associate Fellow	AFHEA 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