

CONTACTS

- **Lecturer in Chemical Engineering**, Institute for Materials and Processes, School of Engineering, University of Edinburgh
Sanderson Building, Robert Stevenson Road, EH9 3FB, UK
- e-mail: ericci@ed.ac.uk - Telephone: +44 (0)751 0849941
- Institutional webpage: <https://eng.ed.ac.uk/about/people/dr-eleonora-ricci>



PROFILE

I am a **Lecturer in Chemical Engineering** at the **University of Edinburgh** and the Principal Investigator of the M2-D2 group (Molecular Modelling and Data-Driven Materials Design). My expertise lies in developing **multiscale and multi-method modelling strategies**, integrating molecular, thermodynamic, and data-driven techniques, to tackle challenges in designing **innovative materials and processes for environmental applications**, such as carbon capture, hydrogen management, biomaterials, membrane separations.

RESEARCH EXPERIENCE

12/2023 – Present **Assistant Professor (Lecturer) in Chemical Engineering**

Institute for Materials and Processes, School of Engineering.
University of Edinburgh, UK.



11/2021 – 11/2023 **Marie Curie Postdoctoral Research Fellow**

Inst. of Informatics and Telecommunications, National Centre for Scientific Research Demokritos, Athens, Greece.

Project ML-MULTIMEM: “**Machine Learning-aided Multiscale Modelling Framework for Polymer Membranes**”.



11/2020 – 10/2021 **Postdoctoral Fellow, Chemical Engineering**

University of Bologna, Italy. Project MuMPol: “*Modelling and Design of Multiphase Polymeric Materials for High Performance Applications Across Multiple Scales*”. Funded by the Dutch Polymer Institute (DPI).



11/2019 – 10/2020 **Postdoctoral Fellow, Chemical Engineering**

University of Bologna, Italy. Project: “*Modelling and characterization of sorption and transport of gases in polymeric membranes for gas separation*”.



INTERNATIONAL EXPERIENCE

09/2024 – 11/2024 **Visiting Researcher**. SINTEF Digital, Oslo, Norway. In the framework of the European Lighthouse to Manifest **Trustworthy and Green AI** Mobility Grant. Project: “*Hybrid AI Model for Mixed-Gas Sorption Upper Bounds*”



11/2019 – 11/2019 **Visiting Researcher**

National Centre for Scientific Research Demokritos, Athens, Greece
HPC Europa 3 Mobility Grant Recipient



06/2017 – 03/2018 **Visiting PhD Student**

National Technical University of Athens, Athens, Greece







EDUCATION

- **Ph.D. in Chemical Engineering** 11/2016 – 10/2019
Department of Civil, Chemical, Environmental and Materials Engineering, University of Bologna, Italy
Thesis: “*Molecular and Thermodynamic Simulations for Pure and Mixed Gas Sorption in Polymeric Membranes*”. Degree obtained: March 2020.
- **Master’s Degree in Chemical and Process Engineering** 09/2014 – 10/2016
University of Bologna – Italy. 110/110, 1st class Honours
Thesis: “*Study of membrane materials for CO₂/CH₄ separation with a combined macroscopic/molecular approach*”.
- **Bachelor’s Degree in Chemical and Biochemical Engineering** 09/2011 – 07/2014
University of Bologna – Italy. 110/110, 1st class Honours.
Thesis: “*Experimental characterization of ceramic materials for membrane contactors*” Work carried out in the framework of an **industrial partnership with Saipem S.p.A.**
- **High School Diploma, Foreign Languages Curriculum** 2006 – 2011
Liceo Classico “L.A. Muratori”, Modena – Italy. 100/100 and Honours.

TEACHING EXPERIENCE

- **Course Organiser**, “Batchwise and Semi-batch Processing”, Univ. of Edinburgh, UK 2024 – 2025
- **Adjunct Professor**, “Molecular Design and Materials Simulation” Univ. of Bologna, Italy 2020 – 2021
- **Teaching Assistant**, University of Bologna, Italy. 2016 – 2020
Thermodynamics for Chemical Engineering (MSc), Thermodynamics for Chemical Engineering (BSc), Introduction to Chemical Engineering, Fluid Dynamics
- **BSc and MSc project Supervisor and Co-Supervisor** 2016 – 2023
I provided training and co-supervision to 16 students from diverse academic backgrounds: BSc and MSc in **Chemical Engineering** (Univ. of Bologna, Italy, University of Edinburgh, UK), MSc in **Biotechnology**, (Univ. of Bologna, Italy), Master of **Artificial Intelligence** (University of Pireus, Greece), MSc in Chemical Engineering (NTUA, Greece), as well as PhD students in Chemical Engineering, in Italy, Greece, and the UK.
- **Summer School Instructor** 09/2019, 01/2020
University of Bologna, Italy - University of Melbourne, Australia. **Blended Summer School on Engineering Processes, Systems & Materials.**

RESEARCH PROJECTS

- 2025 *Reducing greenhouse gas emissions in clinical settings: investigating nitrous oxide separation with membranes.* Edinburgh Research Partnership in Engineering (ERPE); **£4,000**, Principal Investigator 
- 2024 - 2028 CharMPol (*Characterization and Modeling of high-performance polymers for gas barrier applications*) Dutch Polymer Institute; **155,000 €**, co-Principal Investigator. 
- 09-11/2024 ENFIELD: European Lighthouse to Manifest Trustworthy and Green AI- Exchange scheme European Commission, **7,200 €**, Visiting researcher  

- 2021- 2023

ML-MULTIMEM (*Machine Learning-aided Multiscale Modelling Framework for Polymer Membranes*) Marie Skłodowska-Curie Actions **Individual** Fellowships
European Commission, **153,085 €**, Postdoctoral Fellow


- 2023

A Machine Learning Platform for the design of Hydrogen-Ready materials
Royal Society of Edinburgh, Research Workshop Autumn 2022
£ 9,600, co-Principal Investigator


- 2020 - 2024

MuMPol (*Modelling and Design of Multiphase Polymeric Materials for High Performance Applications Across Multiple Scales*)
Dutch Polymer Institute; **140,000 €**, co-Investigator.


- 2021

GHAIA (*Geometric and Harmonic Analysis with Interdisciplinary Applications*). European Commission, **12,000 €**
6-month secondment at the Department of Chemical Engineering at the Massachusetts Institute of Technology (MIT). Due to travel restrictions resulting from the COVID-19 pandemic, it was transformed into a remote secondment.


- 2019 - 2022

ISCRA (Italian Super Computing Resource Allocation) – CINECA
Over 10 million CPU hours (multiple projects: GD-MOF, GS-SCP, MM-PMC, SimPIM, PermCTA)


- 2018 – 2019

HPC-EUROPA3- mobility programme towards High Performance Computing Centres in Europe. Award: **3,500 € + 300,000 CPU hours**



AWARDS AND SCHOLARSHIPS

- 2021

PhD Thesis Award “Excellence Award in Thermodynamics and Transport Properties 2021” from the European Federation of Chemical Engineering: 2nd place
“Patrick Meares” **PhD Thesis Award** from European Membrane Society: runner-up candidate (800€, as a travel grant to present my PhD Thesis at the Euromembrane 2021 conference)
- 2020

Best presentation award for the work “*Multicomponent effects in CO₂/CH₄ separation with glassy membranes*” at the Network Young MemBrains meeting, London, virtual 2020. (300€)
Travel Award from the European Membrane Society to attend ICOM 2020. (300€)
- 2019

Travel Grant from the Membrane Society of Australasia to attend IMSTEC 2020. (700€)
Travel Award from the European Membrane Society to attend EWM 2019. (650€)
- 2018

Travel Award from the European Membrane Society to attend Euromembrane 2018. (420€)
- 2016

Three-year **Scholarship** from the Italian Ministry of Education to pursue the Ph.D. in Chemical and Process Engineering at the University of Bologna (68,000€)
- 2014

Scholarship: Merit-based one-year full tuition fee waiver for the Master’s Degree in Chemical and Process Engineering at the University of Bologna, Italy. (1,500€)
- 2011

Scholarship: Merit-based one-year full tuition fee waiver for the Bachelor’s Degree in Chemical and Biochemical Engineering at the University of Bologna, Italy. (1,300€)

INDUSTRIAL EXPERIENCE AND TRANSLATIONAL RESEARCH

I have actively engaged in collaborations with industrial partners through my research activities. During my PhD, I had the opportunity to collaborate with **Membrane Technology and Research Inc.** (Dr. Tim Merkel), for the characterization and modelling of ternary mixed-gas sorption in polymer membranes, which was being performed then for the first time, on samples provided by our partner, who actively participated in the analysis and interpretation of the results. This successful collaboration resulted in a publication in the Chemical Engineering Journal (IF 16.744).

I participated as co-Investigator and subsequently collaborator in the MuMPol project, that aims at predicting the solubility of gases (CO₂ and hydrogen) in semicrystalline polymers. The project is still ongoing and it is funded by the Dutch Polymer Institute (DPI). The research team periodically reports to and sets interest targets together with the DPI industrial partners participating in MuMPol: **DSM, Shell, Saudi Aramco, Sabic**. This project has yielded two publications [2, 9 in the publications list], with an additional two manuscripts currently in preparation. Moreover, the research activity has been disseminated yearly to the whole industrial and academic partners portfolio of DPI.

As part of the ML-MULTIMEM project, I collaborated with **SciFY - Science for You**, a not-for-profit software company dedicated to the open-source dissemination of scientific results and software. Our collaboration focuses on packaging and distributing the project's code adhering to high-quality standards for reusability and community impact. Additionally, we are working together to create engaging demos and implement communication and outreach initiatives aimed at a wider audience.

INVITED LECTURES AND PRESENTATIONS

- **Invited Seminar at the Complex Network Analysis Group**. NCSR Demokritos, Greece. Title: *"Convolutional Graph Neural Networks for Learning Interactions in Molecular Simulations"*. [Link](#). 21/01/2023
- **Invited Seminar at the European Federation of Chemical Engineering Spotlight Talks Webinar Series**. Title: *"Machine-Learning Methods to Facilitate Coarse-Grained Molecular Simulations"*. [Link](#). +40 participants and ~200 views. 24/11/2022
- **Invited Seminar for the NanoAI Series**, NCSR Demokritos Athens, Greece. [Link](#). Title: *"Coarse Grained Molecular Simulations Facilitated by Machine Learning"*. 20 participants. 21/10/2022.
- **Instructor, 57th NCSR Demokritos Summer School**, Athens, Greece. [Link](#). Title: *"Empowering multi-scale simulations with Machine Learning"*. +100 participants. 12/07/2022
- **Invited Seminar, Research and Industrial Seminars Series – University of Bologna**, Italy. Title: *"Simulation Strategies for the Prediction of the Gas Separation Properties of Polymeric Membranes"*. ~50 participants. [Link](#). 26/03/2021
- **Invited Lecture – University of Melbourne, Australia**, for the class "Recent Advances in Separation Processes", Department of Chemical Engineering. Title: *"Calculation of Solubility in Polymers with Equations of State and Non-Equilibrium models"*. 30/01/2020
- **Invited Seminar – Massachusetts Institute of Technology**, USA. Department of Chemical Engineering, Prof. Zachary Smith Lab. Title: *"Molecular and Macroscopic Simulation Strategies for the Prediction of the Gas Separation Properties of Polymeric Membranes"*. 07/11/2019

CONFERENCES AND EVENTS ORGANISATION

- **Member of the Scientific Committee** - European Symposium on Applied Thermodynamics, Edinburgh, UK, 9-12/06/2024
- **Member of the Organizing Committee and Event Co-chair** Artificial Intelligence in Natural Sciences and Technology Workshop, 12th Hellenic Conference on Artificial Intelligence, Corfu, Greece. 7-9/09/2022
- **Member of the Local Organising Committee**, Blended Summer School on Engineering Processes, Systems and Materials (EPSM), Bologna, Italy. 10-12/09/2019
- **Member of the Local Organising Committee**: International Workshop on Physics of Membrane Processes 2018, Bologna, Italy. 02/09/18

REVIEWING ACTIVITIES

- **Peer Reviewer** for the following Journals:
 - Scientific Reports, Nature
 - Journal of Membrane Science, Elsevier
 - Fluid Phase Equilibria, Elsevier
 - J. of Natural Gas Science and Engineering, Elsevier
 - Journal of Chemical Physics, AIP Publishing
 - Membranes, MDPI, Materials, MDPI
 - Macromolecular Reaction Engineering, Wiley

PROFESSIONAL BODY QUALIFICATIONS AND MEMBERSHIPS

- 03/2017: Accreditation as a **Chartered Chemical Engineer** by the Italian Engineer's Association.
- Member of the European Membrane Society since 2017
- Member of the Hellenic Society of Artificial Intelligence since 2022

PUBLIC ENGAGEMENT AND OUTREACH

- 2022 – 2023 : I am part of the **1000 pioneers for AI in Greece Network**, that organizes technical training and public outreach activities concerning the fundamentals of AI models, their strength and limitations, as well as their utility and relevance for different stakeholders (natural science and humanities researchers, students, NGOs & civil society...).
- 30/09/2022 : I participated in the **European Researchers' Night** at the National Technical University of Athens, Greece. Through computer games and interactive demonstrations, I interacted with children, high school students, and university students, to introduce them to the ideas of molecules, molecular simulations, and supervised machine learning.
- A.Y. 2020-2021 : I participated as a **Mentor in the MyPhDMentor program**, organized by ADI (Italian PhD students and PhD graduates' association) to encourage the exchange of experiences and create a wide intergenerational support network among PhDs, through the creation of mentor/mentee couples between PhD students and PhD graduates from different universities.
- A.Y. 2019-2020: I provided **Guidance and Tutorship** for incoming students in the Bachelor's and Master's Degree in Chemical Engineering, University of Bologna.
- A.Y. 2017-2018 & 2018-2019: I worked at the University of Bologna **Students Recruitment Event** as **Representative** for the Chemical Engineering Programme.

COMMUNITY ENGAGEMENT

- 2023 – 2024: Member of the **Researcher Mental Health Observatory (ReMO) Survey Special Interest Group**. Country Coordinator (Greece) for the dissemination of a large-scale benchmark survey of researchers' mental health in Europe spearheaded the Researcher Mental Health Observatory.
- 2018 – 2023: **Board Member** at **FAIL! – Inspiring Resilience**: Grass-root initiative aimed at increasing awareness about mental well-being in academia, by inviting professors to share experiences of challenging times from their professional or personal lives in a TED talk-style format. I held various executive roles within the association. I served as event organizer, finding and inviting speakers for in-presence and online events, providing guidelines for presentations, chairing sessions and providing technical support. I also served as chief of communication, developing communication strategies, as well as events advertisement campaigns, including evaluation and analytics to optimize communication approaches.

NATIONALITY

- Italian

LANGUAGE SKILLS

- Italian: Native
- English: Proficient (CEFR C2)
- French: Intermediate (CEFR B2)
- German: Intermediate (CEFR B1)
- Greek: Basic (CEFR A2)

INFORMATICS SKILLS

- **Programming languages**: Python, Matlab, Fortran, C++
- **Machine Learning**: PyTorch, scikit-learn
- **Materials Simulation** software: LAMMPS, MAPS, Materials Studio, VMD, ASE, schnetpack
- Familiarity with Windows and **Linux** operating systems.
- Familiarity in the use of **HPC** environments, parallel code execution, **GPU** acceleration.
- Version control and collaborative code development (**Git**)
- Basic knowledge of **Engineering and Process Simulation** software: AutoCad, Phast, Aloha, Aspen Hysys, Ansys Fluent

FULL RESEARCH PUBLICATIONS LIST

Journal Papers: **20**

Citations: **466** (Google Scholar)

Conference Papers: **6**

h-Index: **12** (Google Scholar)

Google Scholar: <https://scholar.google.it/citations?user=ax3B6GIAAAAJ&hl=en&oi=ao>

1. H. Ismaeel, B.D. Marshall, **E. Ricci**, M.G. De Angelis; *A second-order Dry Glass Reference Perturbation Theory for modeling sorption in glassy polymers: applications to systems containing light gases, alcohols, and water vapor.* Fluid Phase Equilibria (2025) 595:114410.
2. R. Di Carlo, **E. Ricci**, M. Minelli; *Comprehensive modelling strategy for gas transport in polymers: Analysis of swelling and non-swelling agents at high pressures.* Fluid Phase Equilibria. (2025) 1;591:114311.
3. K. Papchenko, **E. Ricci**, M.G. De Angelis; *Modelling Across Multiple Scales to Design Biopolymer Membranes for Sustainable Gas Separations: 2-Multiscale Approach.* Polymers. (2024) 30;16(19):2776.
4. **E. Ricci**, M.G. De Angelis; *A perspective on data-driven screening and discovery of polymer membranes for gas separation, from the molecular structure to the industrial performance,* Reviews in Chemical Engineering (2024), 10 (5), 567-600.
5. N.N.R. Ahmad, R. Nasir, **E. Ricci**, C.P. Leo, R. Bahru, S.P. Koh; *Integration of deep eutectic solvent with adsorption and membrane-based processes for CO₂ capture: An innovative approach,* Separation and Purification Technology (2024), 129592.
6. S. Dellis, **E. Ricci**, D.-P. Gerakinis, N. Vergadou, G. Giannakopoulos; *Self-Adaptive Optimization of Coefficients in Multi-Objective Loss Function,* SETN '24: Proceedings of the 13th Hellenic Conference on Artificial Intelligence (2024)
7. D.-P. Gerakinis, **E. Ricci**, G. Giannakopoulos, V. Karkaletsis, D. N. Theodorou, N. Vergadou; *Molecular Simulation of Coarse-grained Systems using Machine Learning,* SETN '24: Proceedings of the 13th Hellenic Conference on Artificial Intelligence (2024)
8. O. Atiq, **E. Ricci**, M. Giacinti Baschetti, M.G. De Angelis; *Molecular Simulations of Hydrogen Sorption in Semicrystalline High-Density Polyethylene: The Impact of the Surface Fraction of Tie-Chains,* Journal of Physical Chemistry B (2024), 128 (11), 2799-2810.
9. H. Ismaeel, D. Gibson, **E. Ricci**, M.G. De Angelis; *Estimating Gas Sorption In Polymeric Membranes From The Molecular Structure: A Machine Learning Based Group Contribution Method For The Non-Equilibrium Lattice Fluid Model (ML-GC-NELF),* Journal of Membrane Science (2024) 691, 122220.
10. **E. Ricci**, N. Vergadou; *Integrating Machine Learning in the Coarse-Grained Molecular Simulation of Polymers,* Journal of Physical Chemistry B (2023), 127 (11), 2302-2322.
11. O. Atiq, **E. Ricci**, M. Giacinti Baschetti, M.G. De Angelis; *Multi-scale modeling of gas solubility in semi-crystalline polymers: bridging Molecular Dynamics with Lattice Fluid Theory,* Fluid Phase Equilibria (2023), 570, 113798.
12. K. Papchenko, **E. Ricci**, M.G. De Angelis; *Modelling across Multiple Scales to Design Biopolymer Membranes for Sustainable Gas Separations: 1—Atomistic Approach,* Polymers (2023) 15 (7), 1805.
13. Q. Qihui, J. Teesdale, L. Hyunhee and K. Rodriguez Mizrahi, **E. Ricci**, F. M. Benedetti, M. G. De Angelis, Z. Smith, *Mixed-Matrix Membranes Formed from Oligomer-Modified Zif-90.* (2023) Preprint, Available at SSRN: <https://ssrn.com/abstract=4380071> or <http://dx.doi.org/10.2139/ssrn.4380071>
14. **E. Ricci**, G. Giannakopoulos, V. Karkaletsis, D. N. Theodorou, N. Vergadou; *Developing Machine-Learned Potentials for Coarse-Grained Molecular Simulations: Challenges and Pitfalls,* SETN '22: Proceedings of the 12th Hellenic Conference on Artificial Intelligence (2022)
15. D. Nasikas, **E. Ricci**, G. Giannakopoulos, V. Karkaletsis, D. N. Theodorou, N. Vergadou; *Investigation of Machine Learning-based Coarse-Grained Mapping Schemes for Organic Molecules,* SETN '22: Proceedings of the 12th Hellenic Conference on Artificial Intelligence (2022)
16. **E. Ricci**, M. Minelli, M.G. De Angelis; *Modelling Sorption and Transport of Gases in Polymeric Membranes across Different Scales: A Review,* Membranes (2022), 12, 9, 857. **Editor's choice paper and Feature paper.**
17. **E. Ricci**, M.G. De Angelis, M. Minelli; *A comprehensive theoretical framework for the sub and supercritical sorption and transport of CO₂ in polymers,* Chemical Engineering Journal (2022), 435, 135013
18. O. Atiq, **E. Ricci**, M.G. Baschetti, M.G. De Angelis; *Modelling solubility in semi-crystalline polymers: a critical comparative review,* Fluid Phase Equilibria (2022), 556, 113412

19. L. Liu, C. M. Doherty, **E. Ricci**, G.Q. Chen, M.G. De Angelis, S. E. Kentish; *The influence of propane and n-butane on the structure and separation performance of cellulose acetate membranes*, Journal of Membrane Science (2021), 638, 119677
20. **E. Ricci**, F.M. Benedetti, A. Noto, T.C. Merkel, J. Jin, M.G. De Angelis; *Enabling Experimental Characterization and Prediction of Ternary Mixed-Gas Sorption in Polymers: C₂H₆/CO₂/CH₄ in PIM-1*, Chemical Engineering Journal (2021), 426, 130715
21. **E. Ricci**, E. Di Maio, M. Degli Esposti, L. Liu, G. Mensitieri, P. Fabbri, S.E. Kentish, M.G. De Angelis; *Towards a systematic determination of multicomponent gas separation with membranes: the case of CO₂/CH₄ in cellulose acetates*, Journal of Membrane Science (2021), 628, 119226
22. **E. Ricci**, F.M. Benedetti, M. E. Dose, M.G. De Angelis, B.D. Freeman, D.R. Paul; *Competitive sorption in CO₂/CH₄ separations: the case of HAB-6FDA polyimide and its TR derivative and a general analysis of its impact on the selectivity of glassy polymers at multicomponent conditions*, Journal of Membrane Science (2020), 612, 118374
23. **E. Ricci**, N. Vergadou, G. Vogiatzis, M.G. De Angelis, D.N. Theodorou; *Molecular Simulations and Mechanistic Analysis of the Effect of CO₂ Sorption on Thermodynamics, Structure, and Local Dynamics of Molten Atactic Polystyrene*, Macromolecules (2020), 53, 10, 3669–3689
24. **E. Ricci**, A. E. Gameda, N. Du, N. Li, M. G. De Angelis, M. D. Guiver, G. C. Sarti; *Sorption of CO₂/CH₄ mixtures in TZ-PIM, PIM-1 and PTMSP: experimental data and NELF-model analysis of competitive sorption and selectivity in mixed gases*, Journal of Membrane Science (2019), 585, 136 – 149
25. **E. Ricci**, M. G. De Angelis; *Modelling Mixed-Gas Sorption in Glassy Polymers for CO₂ Removal: A Sensitivity Analysis of the Dual Mode Sorption Model*, Membranes (2019), 9, 1 – 26. **Editor's choice paper and Cover story paper**. From this paper a **book chapter** was extracted for the volume "Gas Transport in Glassy Polymers" ISSN 2077-0375 <https://doi.org/10.3390/books978-3-0365-0213-7>
26. **E. Ricci**, M. Minelli, M. G. De Angelis; *A multiscale approach to predict the mixed gas separation performance of glassy polymeric membranes for CO₂ capture: the case of CO₂/CH₄ mixture in Matrimid®*, Journal of Membrane Science (2017), 539, 88 – 100