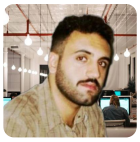

Omar Atiq

Ph.D.

Profile

I am a postdoctoral research assistant at the University of Bologna, Italy. My research is centered on modeling polymeric membranes for packaging and separation applications, such as high-pressure hydrogen storage and transport, as well as the concentration and fractionation of volatile fatty acids (VFAs) in aqueous mixtures using reverse osmosis and nanofiltration. My work employs a systematic methodology that integrates molecular, macroscopic, and multi-scale modeling tools with the ultimate goal of optimizing materials screening and facilitating process scale-up.

Publications

- O. Atiq, E. Ricci, M. Giacinti Baschetti, and M. G. De Angelis, “Molecular Simulations of Hydrogen Sorption in Semicrystalline High-Density Polyethylene: The Impact of the Surface Fraction of Tie-chains,” *J. Phys. Chem. B*, 2024, doi: 10.1021/acs.jpcb.3c07705.
- O. Atiq, E. Ricci, M. Giacinti Baschetti, and M. G. De Angelis, “Multi-scale modeling of gas solubility in semi-crystalline polymers: bridging Molecular Dynamics with Lattice Fluid Theory,” *Fluid Phase Equilib.*, vol. 570, p. 113798, 2023, doi: 10.1016/j.fluid.2023.113798.
- O. Atiq, E. Ricci, M. Giacinti Baschetti, and M. G. De Angelis, “Modelling solubility in semi-crystalline polymers: a critical comparative review,” *Fluid Phase Equilib.*, vol. 556, p. 113412, 2022, doi: 10.1016/j.fluid.2022.113412.
- Ready for submission to the Journal of *Separation and Purification Technology* : O. Atiq, S. Bandini, G. A. Martinez, and L. Bertin, “On the Concentration of Volatile Fatty Acids by Reverse Osmosis and Nanofiltration: membrane characterization and module performance simulation".

Education

Doctor of Philosophy in Chemical Engineering, University of Bologna, Bologna.

November 2020 — March 2024

Thesis: *Multi-scale modeling of gas transport properties in semi-crystalline polymers.*

The research was part of the project 'MuMPol 'funded by the Dutch Polymer Institute (DPI), Netherlands.

supervisor: Prof. Marco Giacinti Baschetti.

co-supervisor: Prof. Maria Grazia De Angelis.

Master degree in chemical and process engineering, University of Bologna, Bologna.

October 2017 — March 2020

Thesis: *Feasibility of membrane processes for Volatile Fatty Acids (VFAs) concentration: data elaboration, modelling, and design.*

Details

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Date / Place of birth

23/03/1995
Rieti, Italy

Nationality

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Links

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Skills

- Microsoft Excel
- LAMMPS
- Matlab
- Aspen HYSYS
- ANSYS FLUENT
- Microsoft PowerPoint
- Open Foam

Languages

- Italian
- English
- Arabic
- French

The thesis was carried out in the context of the *No-AW* (No-Agro Waste) European project, 2016-2020.

grade: 110/110 with honors.

supervisor: Prof. Serena Bandini

★ Visiting research

National Technical University of Athens, Athens, Greece.

February 2023 — June 2023

Molecular simulations of oxygen and hydrogen sorption and diffusion in united atom semi-crystalline High-Density Polyethylene.

supervisor: Prof. Doros N. Theodorou.

University of Edinburgh, UK, Scotland.

September 2022 — December 2022

Experimental measurements of gas sorption and diffusion in polymers.

supervisor: Dr. Enzo Mangano.

★ Conference attendance

European Symposium on Applied Thermodynamics (ESAT), Edinburgh, UK.

June 2024

Oral presentation: "*A multi-scale modeling approach for the prediction of hydrogen transport properties in semi-crystalline polymers*".

AIChE, Orlando, Florida, USA.

November 2023

Oral presentation: "*An Experimental and Theoretical Analysis of Hydrogen Sorption, Diffusion, and Permeation in Semi-crystalline Polymers - Poster presentation: Molecular Modeling of Hydrogen Sorption in Semi-Crystalline High-Density Polyethylene*".

European Symposium on Applied Thermodynamics (ESAT), Graz, Austria.

July 2022

Oral presentation: "*Prediction of hydrogen sorption in semi-crystalline polymers through a multi-scale modeling approach*".

EUROMEMBRANE 2021, Copenhagen, Denmark.

December 2021

Poster presentation: "*Prediction of hydrogen gas sorption in semi-crystalline polymers through a multiscale modeling approach*".

European Symposium on Applied Thermodynamics (ESAT), Paris, France.

July 2021

Poster presentation:" *Multiscale modeling of gas sorption in semi-crystalline polymers*".