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Riccardo Alessandri

Computational Soft Materials Design

Research interests

Computational materials design; soft materials; materials for sustainability; organic electronics; multiscale simulations; coarse-graining; machine learning for chemistry, physics, and materials

Professional Appointments

01/2025–*present* **Assistant Professor**, *Department of Chemical Engineering, KU Leuven*, Belgium

10/2020–12/2024 **(NWO Rubicon) Postdoctoral Fellow**, *Pritzker School of Molecular Engineering, University of Chicago*, USA
Advisor: Prof. Juan J. de Pablo

02/2020–09/2020 **Postdoctoral researcher**, *Zernike Institute for Advanced Materials, University of Groningen*, The Netherlands
Advisor: Prof. Siewert J. Marrink

Education

2014–2019 **Ph.D.** *(cum laude)*, *University of Groningen*, The Netherlands
Dissertation: Multiscale Modeling of Organic Materials: from the Morphology Up [link]
Advisors: Prof. Siewert J. Marrink and Prof. Ria Broer

2012–2014 **M.Sc. in Theoretical Chemistry and Computational Modelling** *(cum laude)*, *University of Groningen*, The Netherlands
Advisors: Dr. Hélène Bolvin, Prof. Ria Broer and Dr. Remco W.A. Havenith

2009–2012 **B.Sc. in Chemistry** *(cum laude)*, *University of Perugia*, Italy
Advisors: Prof. Francesco Tarantelli and Dr. Leonardo Belpassi

Honors and Awards

2024 **Maria Lastra Excellence in Mentoring Award**, *Pritzker School of Molecular Engineering, University of Chicago*, [link]

2024 **Marie Skłodowska-Curie Actions Postdoctoral Fellowship**, *European Commission*, Individual fellowship for 2 years [link]

2023 **Royal Society of Chemistry's 2022 Outstanding Reviewer** (Digital Discovery) [link]

2022 **Paper #17 selected for "Best of the *Advanced* journals 2022"** [link]

2021 **NWO Rubicon Postdoctoral Fellowship**, *Dutch Research Council (NWO)*, Individual fellowship for 2 years [link]

2021 **HPC-Europa3 Transnational Access programme grant**, *European Commission*

2019 **Ph.D. with distinction Cum Laude**, Highest distinction in the Netherlands (top 5%)

2014 **Ph.D. grant NWO Graduate Programme Advanced Materials**, *Dutch Research Council (NWO)*, 4-year Ph.D. funding obtained writing my own research proposal

2012 **Erasmus Mundus Scholarship**, *European Commission*, Complete (2-year) funding for the competitive M.Sc. Theoretical Chemistry and Computational Modeling (TCCM)

2009 **Alessio Trippolini Prize**, *ITTS "A. Volta" Perugia*, for academic achievement [link]

Manuscripts

- M. Ley-Flores, A. Chabbi, **R. Alessandri**, S. Marsden, I. Vettese, S. J. Rowan, J. J. de Pablo, *Numerical Study of Cleavable Bond-Modified Polyethylene for Circular Polymer Design*, arXiv **2024**, arXiv.2404.09341.
- M. Ley-Flores, **R. Alessandri**, S. Najmi, M. Valsecchi, G. Jackson, A. Galindo, L. T. J. Korley, D. G. Vlachos, J. J. de Pablo, *Thermodynamic and Transport Properties of Binary Mixtures of Polyethylene and Higher n-Alkanes from Physics-Informed and Machine-Learned Models*, arXiv **2024**, arXiv.2404.09676.
- C. Zhang, W. Liu, Z. Zhang, H. Liang, S. Shan, **R. Alessandri**, B. T. Diroll, B. Li, G. Wang, T. Fu, J. Yin, W. Lee, Y. Li, R. Yang, P. Guo, J. J. de Pablo, S. Wang, *Host-guest design for stretchable light-emitting polymers reaching an EQE of 20%*, Chemrxiv **2025**, DOI: 10.26434/chemrxiv-2025-h2k0p.
- Y. Wu, **R. Alessandri**, A. E. Coraor, X. Peng, P. F. Zubieta Rico, K. Liebl, K. Trinh, T. R. Sosnick, J. J. de Pablo, *CRANBERRY: An RNA Dynamics Model with Sugar Puckering and Noncanonical Base Pairing*, bioRxiv **2026**, DOI: 10.64898/2026.01.12.699131.

Peer-Reviewed Publications

profile Scholar profile

Highlighted: **JACS Au** (#24), **Macromol.** (#22), **AdvTheorySimul** (#17), **JCTC** (#6), **JACS** (#1)
* denotes corresponding author.

29. G. Zaldivar, R. Dong, J. M. Montes de Oca, G. Sun, **R. Alessandri**, S. N. Patel, P. F. Nealey, J. J. de Pablo, *Water Volume Fraction Governs the Thermodynamics of Water Adsorption of Anion Exchange Membranes*, Macromolecules **2025**, 58, 9972–9982.
28. R. Shrestha, **R. Alessandri**, M. Vögele, P. C. T. Souza, S. J. Marrink, L. Monticelli, *Martini 3 Coarse-Grained Models for Carbon Nanomaterials*, J. Chem. Theory Comput. **2025**, 21, 9035–9053. [Github repo #1] [Github repo #2]
27. B. Yan, **R. Alessandri**, S. J. Marrink, L. S. Lee, J. Liu, *Insight into the Self-Assembly Behaviors of Per- and Polyfluoroalkyl Substances using a "Computational Microscope"*, Environ. Sci. Technol. Lett. **2025**, 12, 626–631. [Nature highlight]
26. F. Grünewald, L. Seute, **R. Alessandri**, M. König, P. C. Kroon, *CGsmiles: A Versatile Line Notation for Molecular Representations Across Multiple Resolutions*, J. Chem. Inf. Model **2025**, 65, 3405. [preprint version] [Github repo]
25. G. P. Pereira, **R. Alessandri**, M. Domínguez, R. Araya-Osorio, L. Grünewald, L. Borges-Araújo, S. Wu, S. J. Marrink, P. C. T. Souza, R. Mera-Adasme, *Bartender: Martini 3 Bonded Terms via Quantum Mechanics-Based Molecular Dynamics*, J. Chem. Theory Comput. **2024**, *20*, 5763. [preprint version] [Github repo]
24. **R. Alessandri**, C.-H. Li, S. Keating, K. T. Mohanty, A. Peng, J. L. Lutkenhaus, S. J. Rowan, D. P. Tabor, J. J. de Pablo, *Structural, Ionic, and Electronic Properties of Solid-State Phthalimide-Containing Polymers for All-Organic Batteries*, JACS Au **2024**, *4*, 2300. [preprint version] [Github repo]
23. P. F. Zubieta Rico, L. Schneider, G. R. Pérez-Lemus, **R. Alessandri**, S. Dasetty, T. D. Nguyen, C. A. Menéndez, Y. Wu, Y. Jin, Y. Xu, S. Varner, J. A. Parker, A. L. Ferguson, J. K. Whitmer, and J. J. de Pablo, *PySAGES: Flexible, Advanced Sampling Methods Accelerated with GPUs*, Npj Comput. Mater. **2024**, *10*, 35. [preprint version] [Github repo]
22. **R. Alessandri**, J. J. de Pablo, *Prediction of Electronic Properties of Radical-Containing Polymers at Coarse-Grained Resolutions*, Macromolecules **2023**, *56*, 3574–3584. [preprint version] [Github repo]
21. W. Liu, C. Zhang, **R. Alessandri**, B. T. Diroll, Y. Li, H. Liang, X. Fan, K. Wang, H. Cho, Y. Liu, Y. Dai, Q. Su, N. Li, S. Li, S. Wai, Q. Li, S. Shao, L. Wang, J. Xu, X. Zhang, D. V. Talapin, J. J. de Pablo, S. Wang, *High-efficiency Stretchable Light-Emitting Polymers from Thermally Activated Delayed Fluorescence*, Nat. Mater. **2023**, *22*, 737–745. [PDF]

20. S. Sami, **R. Alessandri**, J. B. W. Wijaya, F. Grünewald, A. H. de Vries, S. J. Marrink, R. Broer, R. W. A. Havenith, *Strategies for Enhancing the Dielectric Constant of Organic Materials*, J. Phys. Chem. C. **2022**, *126*, 19462–19469.

19. S. J. Marrink, L. Monticelli, M. N. Melo, **R. Alessandri**, D. P. Tieleman, P. C. T. Souza, *Two Decades of Martini: Better Beads, Broader Scope*, WIREs Comput. Mol. Sci. **2023**, *13*, e1620.

18. F. Grünewald, **R. Alessandri**, P. C. Kroon, L. Monticelli, P. C. T. Souza, S. J. Marrink, *Polyply; a Python Suite for Facilitating Simulations of Macromolecules and Nanomaterials*, Nat. Commun. **2022**, *13*, 68. [preprint version] [Github repo]

17. **R. Alessandri***, J. Barnoud, A. S. Gertsen, I. Patmanidis, A. H. de Vries, P. C. T. Souza*, S. J. Marrink*, *Martini 3 Coarse-Grained Force Field: Small Molecules*, Adv. Theory Simul. **2022**, *5*, 2100391. [preprint version] [Github repo] [Selected for "Best of the *Advanced* journals 2022"]

16. I. Patmanidis, **R. Alessandri**, A. H. de Vries, S. J. Marrink, *Comparing Dimerization Free Energies and Binding Modes of Small Aromatic Molecules with Different Force Fields*, Molecules **2021**, *26*, 6069. [preprint version]

15. J. Dong, S. Sami, D. M. Balazs, **R. Alessandri**, F. Jahani, L. Qiu, S. J. Marrink, R. W. A. Havenith, J. C. Hummelen, M. A. Loi, G. Portale, *Fullerene Derivatives with Oligoethylene–Glycol Side Chains: an Investigation on the Origin of their Outstanding Transport Properties*, J. Mater. Chem. C **2021**, *9*, 16217–16225.

14. **R. Alessandri**, F. Grünewald, S. J. Marrink, *The Martini Model in Materials Science*, Adv. Mater. **2021**, *33*, 2008635. [preprint version]

13. P. C. T. Souza, **R. Alessandri**, J. Barnoud, S. Thallmair, I. Faustino, F. Grünewald, I. Patmanidis, H. Abdizadeh, B. M. H. Bruininks, T. A. Wassenaar, P. C. Kroon, J. Melcr, V. Nieto, V. Corradi, H. M. Khan, J. Domański, M. Javanainen, H. Martinez-Seara, N. Reuter, R. B. Best, I. Vattulainen, L. Monticelli, X. Periole, D. P. Tieleman, A. H. de Vries, S. J. Marrink, *Martini 3: a General Purpose Force Field for Coarse-Grained Molecular Dynamics*, Nat. Methods **2021**, *18*, 382–388. [PDF] [Github repo] [News & Views]

12. J. Liu, B. van der Zee, **R. Alessandri**, S. Sami, J. Dong, M. I. Nugraha, A. J. Barker, S. Rousseva, L. Qiu, X. Qiu, N. Klasen, R. C. Chiechi, D. Baran, M. Caironi, T. D. Anthopoulos, G. Portale, R. W. A. Havenith, S. J. Marrink, J. C. Hummelen, L. J. A. Koster, *N-type Organic Thermoelectrics: Demonstration of ZT>0.3*, Nat. Commun. **2020**, *11*, 5694.

11. A. S. Bondarenko, I. Patmanidis, **R. Alessandri**, P. C. T. Souza, T. L. C. Jansen, A. H. de Vries, S. J. Marrink, and J. Knoester *Multiscale Modeling of Molecular Structure and Optical Properties of Complex Supramolecular Aggregates*, Chem. Sci. **2020**, *11*, 11514–11524. [preprint version]

10. B. Kriete, A. S. Bondarenko, **R. Alessandri**, I. Patmanidis, V. V. Krasnikov, T. L .C. Jansen, S. J. Marrink, J. Knoester, M. S. Pshenichnikov, *Molecular versus Excitonic Disorder in Individual Artificial Light-Harvesting Systems*, J. Am. Chem. Soc. **2020**, *142*, 18073–18085.

9. **R. Alessandri***, S. Sami, J. Barnoud, A. H. de Vries, S. J. Marrink*, R. W. A. Havenith*, *Resolving Donor–Acceptor Interfaces and Charge Carrier Energy Levels of Organic Semiconductors with Polar Side Chains*, Adv. Funct. Mater. **2020**, 2004799. [preprint version] [Figshare dataset]

8. P. C. T. Souza, S. Thallmair, P. Conflitti, J. C. Ramírez Palacios, **R. Alessandri**, S. Raniolo, V. Limongelli, S. J. Marrink, *Protein–Ligand Binding with the Coarse-Grained Martini Model*, Nat. Commun. **2020**, *11*, 3714. [Selected in MD simulations and Computational methods in Life Science]

7. S. Sami, **R. Alessandri**, R. Broer, R. W. A. Havenith, *How Ethylene Glycol Chains Enhance the Dielectric Constant of Organic Semiconductors: Molecular Origin and Frequency Dependence*, ACS Appl. Mater. Interfaces **2020**, *12*, 17783–17789.

6. **R. Alessandri**, P. C. T. Souza, S. Thallmair, M. N. Melo, A. H. de Vries, S. J. Marrink, *Pitfalls of the Martini Model*, J. Chem. Theory Comput. **2019**, *15*, 5448–5460. [preprint version]

5. S. Sami, P. A. B. Haase, **R. Alessandri**, R. Broer, R. W. A. Havenith, *Can the Dielectric Constant of Fullerene Derivatives Be Enhanced by Side Chain Manipulation? A Predictive First Principles Computational Study*, J. Phys. Chem. A **2018**, *122*, 3919–3926.

4. **R. Alessandri**, H. Zulfikri, J. Autschbach, H. Bolvin, *Crystal Field in Rare-Earth Complexes: from Electrostatics to Bonding*, Chem. Eur. J. **2018**, *24*, 5538. [PDF]

3. J. Liu, L. Qiu, **R. Alessandri**, X. Qiu, G. Portale, J. Dong, W. Talsma, G. Ye, A. A. Sengrian, P. C. T. Souza, M. A. Loi, R. C. Chiechi, S. J. Marrink, J. C. Hummelen, L. J. A. Koster, *Enhancing Molecular n-Type Doping of Donor-Acceptor Copolymers by Tailoring Side Chains*, Adv. Mater. **2018**, 1704630. [PDF]

2. L. Qiu, J. Liu, **R. Alessandri**, X. Qiu, M. Koopmans, R. W. A. Havenith, S. J. Marrink, R. C. Chiechi, L. J. A. Koster, J. C. Hummelen, *Enhancing Doping Efficiency by Improving Host-Dopant Miscibility for Fullerene-Based n-Type Thermoelectrics*, J. Mater. Chem. A **2017**, *5*, 21234–21241. [PDF]

1. **R. Alessandri**, J. J. Uusitalo, A. H. de Vries, R. W. A. Havenith, S. J. Marrink, *Bulk Heterojunction Morphologies with Atomistic Resolution from Coarse-Grain Solvent Evaporation Simulations*, J. Am. Chem. Soc. **2017**, *139*, 3697–3705. [Github repo]

Book chapters

- **R. Alessandri**, S. Thallmair, C. Gil Herrero, R. Mera-Adasme, S. J. Marrink, P. C. T. Souza, *A Practical Introduction about Martini 3 and Its Application to Protein-Ligand Binding Simulations*, in *A Practical Guide to Recent Advances in Multiscale Modeling and Simulation of Biomolecules*, edited by Y. Wang and R. Zhou (AIP Publishing, Melville, New York, **2023**), pp. 1-1–1-34.

Open-source software and datasets

- (dataset) `Redox-active polymers` [Github repo] (Lead developer)
- (dataset) `Martini 3 small molecule database` [Github repo] (Lead developer)
- (software) `polyply`: generic simulation system and topology builder [Github repo] (Developer)
- (software) `PySAGES`: suite for enhanced sampling techniques [Github repo] (Developer)
- (software) `Bartender`: tool for coarse-grained model parametrization [Github repo] (Developer)
- (dataset) Organic photovoltaic morphologies and force fields [Figshare dataset] (Lead developer)
- (software) Simulated solvent evaporation for soft matter blends [Github repo] (Lead developer)

Selected Talks

2026 (**invited**) *"Molecular dynamics simulations of soft materials"*, Workshop "Towards Biointegrable Soft Matter: from Fundamentals to Applications", Leuven, Belgium (*upcoming*)

2025 (**invited**) *"Modeling structure, ions, and electrons in mixed conducting polymers"*, Seminar at the Laboratory of Organic Electronics, Norrköping, Sweden

2025 (**invited**) *"Multiscale Simulations of Polymeric Mixed Ionic-Electronic Conductors"*, Telluride Workshop 'Fundamentals of Organic and Hybrid Mixed Ionic and Electronic Conductors', Telluride, USA [link]

2025 (**invited**) *"Small Molecule Parametrization"*, Martini Workshop 2025, Groningen, The Netherlands

2025 *"Integrating Electronic Structure into Coarse-Grained Simulations of Electron-Conducting Polymers"*, TCCM 25$^{\text{th}}$ Anniversary Workshop, San Sebastian, Spain

2025 (**invited**) *"Integrating Electronic Structure into Mesoscale Polymer Simulations"*, European Polymer Congress 2025 (EPF 2025), Groningen, The Netherlands

2025 *"Multiscale Polymer Informatics"*, Una Europa-KU Leuven 'Future of Materials Symposium', Leuven, Belgium

2024 (**invited**) *"Multiscale Modeling of Radical-Containing Polymeric Mixed Conductors"*, Northwestern Theoretical Chemistry Seminar Series, Northwestern University, Evanston, USA

2024 *"Structure-Property Relationships in Mixed Ionic-Electronic Conductors via Machine Learning-Enhanced Multiscale Modeling"*, APS March Meeting 2024, Minneapolis, USA [abstract]

2024 (**invited**) *"Multiscale Modeling for the Design of Functional Soft Materials"*, University of Turku, Turku, Finland

2024 (**invited**) *"Multiscale Modeling for the Design of Functional Soft Materials"*, KU Leuven, Leuven, Belgium (virtual)

2023 *"Machine Learning to Bridge Scales in the Multiscale Modeling of Radical-Containing Polymers"*, 2023 MRS Fall Meeting, Boston, USA [abstract]

2023 (**invited**) *"Coarse-Grained Modeling of Biomolecules, Soft Materials, and Electronic Structure"*, International Conference in Bioinformatics, Simulation, and Modeling (iCBSM4), Talca, Chile

2023 *"Multiscale Simulations of Solid-State Redox-Active Polymers for Energy Storage"*, 2023 AIChE Annual Meeting, Orlando, USA [abstract]

2023 (**invited**) *"Multiscale Modeling for the Design of Functional Soft Materials"*, University of Turku, Turku, Finland (virtual)

2023 (**invited**) *"Martini Coarse-Grained Model: Past, Present and Future"*, BASF SE, virtual

2023 (**invited** (in place of J.J. de Pablo)) *"Polymer Design and Characterization in the Era of Machine Learning"*, Frontiers in Polymer Science 2023, Gothenburg, Sweden

2023 (**invited**) *"Physics-Based and AI-Driven Design of Functional Soft Materials"*, Delft University of Technology, Delft, The Netherlands

2023 *"Morphology-Electronic Structure Relationships in Radical-Containing Polymers for All-Organic Batteries"*, ACS Spring 2023, Indianapolis, USA [abstract]

2023 (**invited**) *"Machine Learning-Enhanced Multiscale Modeling of Soft Electronic Materials"*, Seminar at Eindhoven University of Technology, Eindhoven, The Netherlands

2023 (**invited**) *"Machine Learning-Enhanced Multiscale Modeling of Soft Electronic Materials"*, Zernike Seminar, University of Groningen, Groningen, The Netherlands

2022 *"Machine Learning-Enabled Prediction of Electronic Properties of Radical Polymers at Coarse-Grained Resolutions"*, 2022 AIChE Annual Meeting, Phoenix, USA [abstract]

2022 (**invited** (in place of S.J. Marrink)) *"Coarse-Graining with Martini 3: from Small Molecules to Soft Materials"*, CECAM workshop "Development of CG Models", Lyon, France (*postponed from 2020 due to pandemic; declined due to travel constraints*)

2022 (**invited**) *"Martini in Materials Science"*, 2$^{\text{nd}}$ Martini Developers Meeting, Saint Paul's Bay, Malta

2022 *"Predicting Electronic Properties of Macromolecular Radicals at Coarse-Grained Resolutions"*, ACS Fall Meeting 2022, Chicago, USA [abstract]

2022 *"Connecting Electronic Structure and Morphology to Model Organic Electronic Materials"*, Int'l. Symposium on Flexible Organic Electronics (ISFOE) 2022, virtual

2022 *"Electronic Properties of Radical-Containing Polymers at Coarse-Grained Resolutions"*, Midwest Thermodyn. & Stat. Mech. 2022 @ Purdue University, West Lafayette, USA

2022 (**invited**) *"Towards Computationally-Driven Design of Functional Soft Materials"*, Seminar at the University of Amsterdam, Amsterdam, The Netherlands

2022 *"Predicting Electronic Properties of Radical Polymers at Coarse-Grained Resolutions"*, APS March Meeting 2022, Chicago, USA [abstract]

2021 *"Connecting Electronic Structure and Mesoscopic Scales to Model Organic Photovoltaics"*, nanoGe Fall Meeting 2021, virtual [slides]

2021 *"The Martini Coarse-Grained Model for Materials Modeling"*, European Materials Research Society 2021 Fall Meeting, virtual [slides]

2021 (**invited**) *"Martini 3 Coarse-Grained Force Field: Small Molecules"*, Martini Coarse-Graining Workshop 2021, virtual [▶ video] [slides]

2019 *"Martini 3.0: a Matter of Size"*, 1st Martini Developers Meeting, Faro, Portugal

2018 *"Computational Design of Organic Blends"*, Dutch physics national conference "Physics@Veldhoven", Veldhoven, The Netherlands

2017 *"Soft Matter Morphologies with Atomistic Resolution from Coarse-Grain Solvent Evaporation Simulations"*, CECAM workshop "Multiscale Modeling of Organic Semiconductors", Grenoble, France

2017 (**invited**) *"Blends for Organic Photovoltaics"*, Martini Coarse-Graining Workshop 2017, Groningen, The Netherlands [slides]

2017 *"Bulk Heterojunction Morphologies with Atomistic Resolution from Coarse-Grain Solvent Evaporation Simulations"*, Conference "Next-Gen III: PV materials", Groningen, The Netherlands

2017 *"Bulk Heterojunction Morphologies with Atomistic Resolution from Coarse-Grain Solvent Evaporation Simulations"*, Lorentz Center workshop on "Structured Soft Interfaces", Leiden, The Netherlands

Funding

2025 *"High-Throughput Polymer Simulations"* (Lead)
LUMI HPC Preparatory Project - **250k CPU h + 12.5k GPU h**
Role: Lead PI - Conceived, wrote, and submitted.

2024 *"Electronic Mesoscale Modeling of Organic Mixed Conductors"* (Lead)
Marie Skłodowska-Curie Actions Fellowship - **€200k/2 years** (*relinquished*) [link]
Role: Lead PI - Conceived, wrote, and submitted.

2021 *"Designing Battery Materials: Smart Navigation through Polymer Haystacks"* (Lead)
NWO Rubicon Postdoctoral Fellowship - **€134k/2 years** [link]
Role: Lead PI - Conceived, wrote, and submitted.

2021 *"Embedded Excited State Dynamics for Organic Photovoltaics"* (Lead)
HPC-Europa3 Transnational Access programme - **168k CPU h** (*relinquished*)
Role: Lead PI - Conceived, wrote, and submitted.

2020–2024 Research Computing Center (RCC) Semiannual Cluster Allocation
University of Chicago - **4.0M CPU h** (aggregated)
Role: Conceived subproject, contributed to writing.

2015–2019 SURFSara, Dutch National Supercomputer Cartesius Annual Allocation
University of Groningen - **10M CPU h** (aggregated)
Role: Conceived subproject, contributed to writing.

2014 *"Multiscale Modelling of Organic Photovoltaics"* (Lead)
NWO Graduate Programme Advanced Materials - **€200k/4 years**
Role: Lead PI - Conceived, wrote, and submitted.

Teaching and Pedagogy

2025-2026 Co-Lecturer, Chemical Statistical Mechanics (M.Sc.), KU Leuven

2025-2026 Lecturer, Analytical Chemistry (B.Sc.), KU Leuven

2025-2026 Supervisor, Engineering Experience 3 (B.Sc.), KU Leuven

2025 Lecturer and tutorial coordinator, Martini Workshop 2025, University of Groningen [tutorial]

2023 Lecturer and tutorial coordinator, "Modeling Biomolecules and Soft Materials with the Martini Coarse-Grained Approach", iCBSM4, Talca, Chile

2022 Teaching assistant, PySAGES hands-on tutorial, Humboldt University of Berlin

2021 Lecturer and tutorial coordinator, Martini Workshop 2021, virtual [▶ lecture]

2018-2019 Teaching assistant, Physical Chemistry I (B.Sc.), University of Groningen

2017-2018 Teaching assistant, Quantum chemistry (B.Sc.), University of Groningen

2017-2018 Teaching assistant, Physical Chemistry I (B.Sc.), University of Groningen

2016 Teaching assistant, Molecular Dynamics (M.Sc.), University of Groningen
2016-2017 Teaching assistant, Physical Chemistry I (B.Sc.), University of Groningen
2016 University of Groningen "Teaching for PhD Students" course certificate
2015-2016 Teaching assistant, Physical Chemistry I (B.Sc.), University of Groningen
2014-2015 Teaching assistant, Physical Chemistry I (B.Sc.), University of Groningen

Mentoring and Supervision

- **KU Leuven**, Leuven, Belgium:

11/2025–*present* Behrad Jandaghian Bidgoli, Ph.D. student (Co-supervisor)
10/2025–*present* Besa Mulaj Krasniqi, Ph.D. student (Main supervisor)
09/2025–*present* Alireza Mirzaalipour, Ph.D. student (Main supervisor)
03/2025–05/2025 Luis Gonzalo Espinoza Arcos, Visiting Ph.D. student (Co-supervisor)
02/2025–06/2025 Besa Mulaj Krasniqi, M.Sc. student (Main supervisor)
01/2025–06/2025 María Ley-Flores, Visiting Ph.D. student (Co-supervisor)

- **University of Chicago**, Chicago, USA:

05/2024–12/2024 Kha Trinh, Ph.D. student (Co-supervisor)
05/2024–08/2024 Luis Gonzalo Espinoza Arcos, Visiting Ph.D. student (Co-supervisor)
04/2021–12/2024 María Ley-Flores, Ph.D. student (Co-supervisor)
10/2020–12/2024 Yiheng Wu, Ph.D. student (Co-supervisor)
10/2020–12/2024 Cheng Zhang, Ph.D. student (Co-supervisor)

- **University of Groningen**, Groningen, The Netherlands:

Co-supervision of more than 8 M.Sc. and B.Sc. students.

Service and Outreach

2025–*present* Member of the Faculty of Engineering Technology Council, KU Leuven
2025–*present* Member of the Chemical Engineering Department Council, KU Leuven
2025–*present* M.Sc. thesis assessor at KU Leuven: Chemical Engineering Department (1), Chemistry Department (3);
total of **4 assessments**.
2024–*present* Grant/Application Reviewer for Research Foundation Flanders (FWO), NExT (Nantes Excellence Trajectory) Junior Talent Application;
total of **3 reviews**.
2020–*present* Reviewer for ACS (Biomacromolecules, Chemistry of Materials, Journal of Chemical Theory and Computation, Macromolecules, Journal of Chemical Information and Modeling), AIP (Applied Physics Letters, APL Materials, Journal of Chemical Physics), ML4Materials @ International Conference on Learning Representation (ICLR), IOP (Journal of Physics: Materials), Machine Learning and the Physical Sciences Workshop (MLPS at NeurIPS), RSC (Digital Discovery, Chemical Science), Taylor & Francis (Molecular Physics); Springer (Nature Communications, Cellulose);
total of **53 reviews** [Web of Science peer-review profile].
2023–*present* Board member Martini Force Field Initiative [link]
2025 Doctoral defense committee of L. Galleni, KU Leuven, Belgium
2020 Doctoral defense committee of I. Patmanidis, University of Groningen, The Netherlands
2019 One of the two organizers of the "1st Martini Developers Meeting".
2015–2018 One of the four organizer of the annual "Dutch MD Day" meeting.