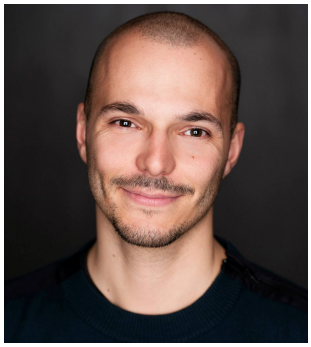

Enrico Riccardi, Ph.D.

Norwegian University of Science and Technology (NTNU)
Department of Applied Theoretical Chemistry, Høgskoleringen 5
7011 Trondheim, Norway
Phone: +47 942 96055
Email: enrico.riccardi@ntnu.no

Birth date and place

16.05.1982, Biella, Italy

Competences

Molecular Dynamics, QM, QM/MM
Transport in porous layers (Ion exchange chromatography)
Rare Event Simulation Methods (reaction kinetics)
Mechanical description of soft matter interphases
Multi-scale modelling (from molecular simulations to continuous mechanics)

Education

Ph.D., Chemical Engineering, 2009.
Department of Chemical and Biological Engineering,
Missouri University of Science and Technology, Mo, USA.

Master Degree, Chemical Engineering, 2006.
Department of Chemical Engineering,
Politecnico di Torino (Technical University of Turin), Turin, IT

Visiting Scholar (Erasmus), 2004.
Department of Textile et fibres,
L'Université de Haute-Alsace, Mulhouse, Cedex, FR

Bachelor Degree, Textile Engineering, 2004.
Department of Chemical Engineering,
Politecnico di Torino (Technical University of Turin), Turin, IT

Work Experience

Researcher (Forsker), 2017 - current (January - June 2019 33% position)
Chemistry Department, NTNU, Trondheim, NO.

Lecturer (**Docent**) January - June 2019 - 67% position
Chemistry Department, NTNU, Trondheim, NO.

Post Doc, 2014-2016,
Chemistry Department, group of Prof. T. van Erp, NTNU, Trondheim, NO.

Post Doc, 2013,
Chemical Engineering Department, group of Prof. J. Sjöblom, NTNU, Trondheim, NO.

Post Doc, 2009-2012,
Chemistry Department, group of Prof. F. Mueller-Plathe, TUD, Darmstadt, DE.

Awards and Scholarship

Best Bachelor Thesis, 2004
Cittá Studi, Politecnico di Torino (Technical University of Turin)
Recipient of Scholarship

Best 2nd year Student, 2003,
Cittá Studi, Politecnico di Torino (Technical University of Turin),
Recipient of Scholarship.

Best report for the "Textile and Health Association", 2003,
Textile Materials for Cardiovascular Applications,
Recipient of Scholarship.

Best 1st year Student, 2002,
Cittá Studi, Politecnico di Torino (Technical University of Turin),
Recipient of Scholarship.

Funding

Workshop/school: Lorentz Center, Leiden, 2019
title: Rare Events via PyRETIS
aim: constructing a community of users of the developed theory and computational tools
Role: Main proposer and organizer
Funding: 50k Euros for a two weeks workshop

Industrial application of research results, 2018
in collaboration with CRIOFARMA, Turin, IT
Project: Impianto Industriale di Ricerca e Sviluppo Prodotti Alimentari Liofilizzazti ad Alta Tecnologia / Research on industrial plants and freezedried food products with Advanced Technology
Role: Consultant. Designer of the scientific/research section of the project
Funding: 5M Euros project for 3 years

PETROMAKS 2, 2017
group of Prof. T. van Erp, NTNU, Trondheim, NO
Project: A multidisciplinary approach to characterize coalescence in petroemulsions
Role: Main proposer and designer of the whole scientific and administrative plan of the project
Funding: 14M Nok in 4 years

Olav Thon foundation, 2016
group of Prof. T. van Erp, NTNU, Trondheim, NO
Project: Komplekse matematiske algoritmer oven-fra-og-ned: Monte Carlo-metoder for stigenerering forklart av studenter til studenter
Role: co-designer of the pedagogical approach
Funding: 3M Nok in 3 years

HRSMC Fellowship, mobility grant, 2017
group of Prof. J. Vreede, UvA, Amsterdam, NL
Project: Selective binding of H-NS to DNA
Role: Recipient and visitor, initiator and co-designer of the project
Funding: 5K Euro for a 3 months visiting period

Funding

EBSA Bursaries, mobility grant, 2017
group of Prof. E. Papaleo, Danish Cancer Society, Copenhagen, DK
Project: Advanced Transition Interface Sampling
to study conformational changes in Cyclophilin A
Role: Recipient and visitor, initiator and co-designer of the project
Funding: 2K Euro for a 2 months visiting period

HRSMC Fellowship, mobility grant, 2016
group of Prof. J. Vreede, UvA, Amsterdam, NL
Project: Simulating the binding modes of H-NS to DNA
Role: Recipient and visitor, initiator and co-designer of the project
Funding: 5K Euro for a 3 months visiting period

Teaching and Advisoring

Teaching assistant, Thermodynamics
TUD, Darmstadt, DE, 2011

Teaching assistant, Computational Chemistry
TUD, Darmstadt, DE, 2012

Lecturer, Chemometrics
NTNU, Trondheim, NO, 2019

Co-advisor Ph.D. candidate, NTNU, Ola Aarøen 2017 – in progress
(main advisor: Prof. Marit Sletmoen)
Co-advisor Ph.D. candidate, NTNU, Anastasia Maslechko 2015 – in progress
(main advisor: Prof. Titus van Erp)
Co-advisor Ph.D., NTNU, Mahmoud Moqadam 2014 – 2016
(main advisor: Prof. Titus van Erp)
Co-advisor Ph.D., NTNU, Aleksandar Mehandzhiyski 2013-2016
(main advisor: Prof. Brian Grimes)
Co-advisor Ph.D., NTNU, Karina Kovalchuk, 2012-2014
(main advisor: Prof. Brian Grimes)

Various tutorial and teaching to master students

Conferences Workgroups

Regular attendance, twice a year, to international conferences
Continous attendance and organization
of local, national and international work groups

Institutional Roles

Boad Member DION, Trondheim, NO, 2016-2018
(Ph.D. and Post Doc interest organization) http://org.ntnu.no/dion/about-us/
Main achievements: organization of several social events,
support for several Ph.D. students with advisor miss-guidance
coordination with companies to supply housing for visiting researchers at NTNU

Institutional Roles

Boad Member, SiN, Norway, 2016-2018
Vice-President, SiN, Norway, 2018-2019
(national Ph.D. and Post Doc interest organization) http://stipendiat.no/

Work Group Coordinator, Open Access/Open Science - EuroDoc, 2017,2018
(European Council of Doctoral Candidates and Junior Researchers)
Main achievements: Preparation

Interactions with public

Main Organiser and panel leader of DION+ProtestPub, Trondheim, NO, 9.11.2016
panel discussion: 'Homeless Academics'

Organiser, via SiN, of EuroDoc conference, Oslo, NO 27-28.4.2017
conference theme: "Open Access"

Proposer and Organizer of the shool "Transition Path Sampling Simulations via PyRETIS"
to be held at the Lorentz Center, Leiden, NL in 2019 (proposal under approval)

Commission of Trust

Scientific Advisory Board for selection of Ph.D. candidate, Trondheim, NO, 2015
selection of Ph.D. candidate, Chemistry Department, NTNU

Scientific Advisory Board, Trondheim, NO, 2017
selection of Ph.D. candidate, Biotecnology Department, NTNU

Languages

Italian (Native)
English (advanced)
French (medium-advanced)
German (medium)
Spanish (medium)
Norwegian (medium)

References

Prof. Titus van Erp - former Group Leader
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Prof. Henrik Koch
Department of Physical Chemistry,
Normale di Pisa
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Ass Prof. Jocelyne Vreede
Faculteit der Natuurwetenschappen,
Wiskunde en Informatica Van 't Hoff Institute for Molecular Sciences
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Publications list of Peer Reviews Journal Articles and Books

1. E. Riccardi, J.-C. Wang, and A. I. Liapis, "Rational surface design for molecular dynamics simulations of porous polymer adsorbent media," *The Journal of Physical Chemistry B*, vol. 112, no. 25, pp. 7478–7488, 2008

2. E. Riccardi, J.-C. Wang, and A. I. Liapis, "Porous polymer adsorbent media constructed by molecular dynamics modeling and simulations: the immobilization of charged ligands and their effect on pore structure and local nonelectroneutrality," *The Journal of Physical Chemistry B*, vol. 113, no. 8, pp. 2317–2327, 2009

3. E. Riccardi, J.-C. Wang, and A. Liapis, "The design by molecular dynamics modeling and simulations of porous polymer adsorbent media immobilized on the throughpore surfaces of polymeric monoliths," *Journal of chromatographic science*, vol. 47, no. 6, pp. 459–466, 2009

4. E. Riccardi, J.-C. Wang, and A. I. Liapis, "Protein adsorption in porous adsorbent particles: A multiscale modeling study on inner radial humps in the concentration profiles of adsorbed protein induced by nonuniform ligand density distributions," *Journal of separation science*, vol. 32, no. 18, pp. 3084–3098, 2009

5. E. Riccardi and A. I. Liapis, "Adsorption of a single protein interacting with multiple ligands: Inner radial humps in the concentration profiles induced by non-uniform ligand density distributions," *Journal of separation science*, vol. 32, no. 23-24, pp. 4059–4068, 2009

6. E. Riccardi, "Rational construction by molecular dynamics modeling and simulations of porous adsorbent media for bioseparation," *Ph.D. Thesis*, pp. 1–300, 2009

7. A. I. Liapis, E. Riccardi, and J.-C. Wang, "Effects on the dynamic utilization of the adsorptive capacity of chromatographic columns induced by non-uniform ligand density distributions," *Journal of separation science*, vol. 33, no. 17-18, pp. 2749–2756, 2010

8. E. Riccardi, J.-C. Wang, and A. Liapis, "A molecular dynamics study on the transport of a charged biomolecule in a polymeric adsorbent medium and its adsorption onto a charged ligand," *The Journal of chemical physics*, vol. 133, no. 8, p. 084904, 2010

9. E. Riccardi, M. C. Böhm, and F. Müller-Plathe, "Molecular dynamics method to locally resolve poisson's ratio: Mechanical description of the solid–soft-matter interphase," *Physical Review E*, vol. 86, no. 3, p. 036704, 2012

10. L. Mammen, X. Deng, M. Untch, D. Vijayshankar, P. Papadopoulos, R. Berger, E. Riccardi, F. Leroy, and D. Vollmer, "Effect of nanoroughness on highly hydrophobic and superhydrophobic coatings," *Langmuir*, vol. 28, no. 42, pp. 15005–15014, 2012

11. E. Riccardi, J.-C. Wang, and A. I. Liapis, "Molecular modeling of polymeric adsorbent media: The effects of counter-ions on ligand immobilization and pore structure," *Journal of separation science*, vol. 35, no. 22, pp. 3073–3083, 2012

12. E. Riccardi, J.-C. Wang, and A. I. Liapis, "Modeling the construction of polymeric adsorbent media: Effects of counter-ions on ligand immobilization and pore structure," *The Journal of chemical physics*, vol. 140, no. 8, p. 084901, 2014

13. K. Kovalchuk, E. Riccardi, A. Mehandzhiyski, and B. Grimes, "Aggregates of poly-functional amphiphilic molecules in water and oil phases," *Colloid Journal*, vol. 76, no. 5, pp. 564–575, 2014

14. E. Riccardi, M. C. Böhm, and F. Müller-Plathe, "Molecular dynamics approach to locally resolve elastic constants in nanocomposites and thin films: Mechanical description of solid-soft matter interphases via young's modulus, poisson's ratio and shear modulus.," *European Physical Journal E–Soft Matter*, vol. 37, no. 10, pp. 1292–8941, 2014

15. E. Riccardi, K. Kovalchuk, A. Mehandzhiyski, and B. Grimes, "Structure and orientation of tetracarboxylic acids at oil–water interfaces," *Journal of Dispersion Science and Technology*, vol. 35, no. 7, p. 103, 2014

16. K. Kovalchuk, E. Riccardi, and B. Grimes, "Multiscale modeling of mass transfer and adsorption in liquid–liquid dispersions. 1. molecular dynamics simulations and interfacial tension prediction for a mixed monolayer of mono-and tetracarboxylic acids," *Industrial & Engineering Chemistry Research*, vol. 53, no. 29, pp. 11691–11703, 2014

17. K. Kovalchuk, E. Riccardi, and B. Grimes, "Multiscale modeling of mass transfer and adsorption in liquid–liquid dispersions. 2. application to calcium naphthenate precipitation in oils containing mono-and tetracarboxylic acids," *Industrial & Engineering Chemistry Research*, vol. 53, no. 29, pp. 11704–11719, 2014

18. A. Y. Mehandzhiyski, E. Riccardi, T. S. van Erp, H. Koch, P.-O. Åstrand, T. T. Trinh, and B. A. Grimes, "Density functional theory study on the interactions of metal ions with long chain deprotonated carboxylic acids," *The Journal of Physical Chemistry A*, vol. 119, no. 40, pp. 10195–10203, 2015

19. A. Y. Mehandzhiyski, E. Riccardi, T. S. van Erp, T. T. Trinh, and B. A. Grimes, "Ab initio molecular dynamics study on the interactions between carboxylate ions and metal ions in water," *The Journal of Physical Chemistry B*, vol. 119, no. 33, pp. 10710–10719, 2015

20. M. Moqadam, E. Riccardi, T. T. Trinh, P.-O. Åstrand, and T. S. van Erp, "A test on reactive force fields for the study of silica dimerization reactions," *The Journal of chemical physics*, vol. 143, no. 18, p. 184113, 2015

21. T. S. van Erp, M. Moqadam, E. Riccardi, and A. Lervik, "Analyzing complex reaction mechanisms using path sampling," *Journal of Chemical Theory and Computation*, vol. 12, no. 11, pp. 5398–5410, 2016

22. M. Moqadam, E. Riccardi, T. T. Trinh, A. Lervik, and T. S. van Erp, "Rare event simulations reveal subtle key steps in aqueous silicate condensation," *Physical Chemistry Chemical Physics*, vol. 19, pp. 13361–13371, 2017

23. E. Riccardi, O. Dahlen, and T. S. van Erp, "Fast decorrelating monte carlo moves for an efficient transition path sampling," *Journal Physical Chemistry Letters*, vol. 8, no. 18, pp. 4456–4460, 2017

24. A. Lervik, E. Riccardi, and T. S. van Erp, "Pyretis: A well-done, medium-sized python library for rare events," *Journal of Computational Chemistry*, vol. 38, no. 28, pp. 2439–2451, 2017

25. M. Moqadam, A. Lervik, E. Riccardi, V. Venkatraman, B. K. Alsberg, and T. S. van Erp, "Local initiation conditions for water autoionization," *Proceedings of the National Academy of Sciences*, vol. 115, no. 20, pp. E4569–E4576, 2018

26. A. Maslechko, T. Verstraelen, T. S. van Erp, and E. Riccardi, "Multiscale partial charge estimation on graphene for neutral, doped and charged flakes," *Physical Chemistry Chemical Physics*, vol. 20, no. 31, pp. 20678–20687, 2018

27. E. Riccardi, E. C. van Mastbergen, W. W. Navarre, and J. Vreede, "Predicting the mechanism and rates of H-NS binding to AT-rich DNA," *Public Library of Science*, p. accepted for publication Jannuary, 2019

28. E. Riccardi and T. Tichelkamp, "Effects of calcium/sodium ratio on hydrocarbon-water interfaces in the presence of anionic surfactants," *Journal of Rheology*, p. submitted for publication in Jan, 2019

29. E. Riccardi, S. Pantano, and R. Potestio, "Envisioning data sharing for the biocomputing community," *Journal of the Royal Society Interface*, p. submitted for publication in Jan, 2019