

UNIVERSITÀ DEGLI STUDI DI MILANO

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Alfonso Gautieri

CURRICULUM VITAE

INFORMAZIONI PERSONALI (NON INSERIRE INDIRIZZO PRIVATO E TELEFONO FISSO O CELLULARE)

COGNOME	GAUTIERI
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DATA DI NASCITA	24 MAGGIO 1981

Personal Information

Date of birth: May 24, 1981
Place of birth: Milan, Italy
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Current Position

2017-present	Politecnico di Milano (Italy)	Assistant Professor
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Previous Scientific Positions

2015-2017	Politecnico di Milano (Italy)	Post-doc
2014-2015	ETH Zurich (Switzerland)	Post-doc
2011-2014	Politecnico di Milano (Italy)	Post-doc
2010-2011	Massachusetts Institute of Technology (USA)	Post-doc
2009-2010	Politecnico di Milano (Italy)	Post-doc

Education

2009	Ph.D., Bioengineering, Politecnico di Milano (Italy) Dissertation title "Multi-scale Computational Investigation of Tendon and Bone Hierarchical Structure and Collagen-related Diseases". Advisor: Prof. Alberto Redaelli
2005	M.S. (grade 110/110 <i>cum laude</i>), Bioengineering, Politecnico di Milano (Italy)

Dissertation title “Investigation of the permeability of bio-artificial membranes using molecular simulation techniques”

Advisor: Prof. Alberto Redaelli

2003

B.S., Bioengineering, Politecnico di Milano (Italy)

Research Interests

I coordinate the Biomolecular Engineering Laboratory at Politecnico di Milano which is focused on the development of *in silico* methods to engineer proteins and peptides. I have extensive experience in the use and development of computational methods for in-depth investigations of proteins structure, protein rational design, protein-ligand docking, molecular dynamics simulations, free energy calculations, homology modelling, high-throughput virtual screening, structure-based design, machine learning for data analysis. I also have experience in complementary experimental techniques, such as protein expression, purification, crystallography, and electron density map solving of protein structure in complex with small molecules.

My main research interest concern the characterization and redesign of Amadoriase enzymes with the aim of developing protein deglycating enzymes, to be used as therapeutic proteins, diagnostic tools for diabetes, or for food preservation. Further research interests involve the development of large-scale molecular modeling tools to design self-assembling peptides for nano(bio)technological applications.

My work has been presented in more than 30 peer reviewed papers (17 as first author, 8 as corresponding and/or last author), 3 book chapters and more than 20 proceedings for international meetings. My work has been published in high-rank journals such as Nature Communications and Nano Letters. I am currently PI of a CARIPLO Foundation grant on biomedical research and I participated in several funded projects from Italian and European agencies. Here are presented the most relevant research lines in which I am currently involved.

Development of engineered enzymes. Blood glucose can alter functional proteins through the formation of so-called Advanced Glycation End-products (AGEs). AGEs accumulation is particularly severe in the elderly and in diabetic patients. The glycation process, albeit slow, is cumulative and irreversible and it affects all proteins indiscriminately. It has been related to a long series of adverse clinical outcomes including arterial stiffening, nephropathy, and retinopathy. However, there are currently no effective ways of preventing AGEs formation. A promising strategy to prevent protein glycation involves the use of Amadoriase enzymes, naturally occurring enzymes that are able to cleave glycated amino acids, but are inactive on whole proteins. Starting from the Amadoriase I crystal structure and extensive computational characterization that we have recently provided, I am developing a combined *in silico*-experimental approach to rationally design protein-deglycating Amadoriase enzymes. These engineered enzymes will be able to cleave glycation products on larger molecules (proteins or protein fragments), thus providing a viable therapeutic tool against AGEs-induced tissue stiffening and aging. Additionally, the proposed innovative strategy for enzyme design is expected to boost knowledge-based design of different biological nanomachines for diverse applications, and thus with huge potential impacts in several areas such as health, agriculture, food processing and fuel industry. This research is currently funded by CARIPLO foundation (“Biomedical research conducted by young researchers”, Principal Investigator). On the topic I submitted an ETN proposal as Coordinator (Call 2020).

Computer-aided design of Self-Assembling Peptides. Self-assembling peptides (SAPs) consist of short peptides able to form highly organized nanostructures. My research in this area consists in the use and development of large-scale molecular modeling tools to design SAPs. Coarse grain and classical atomistic molecular dynamics simulations of the peptides are performed in order to assess the key properties of the peptides such as solubility, propensity to aggregation and driving interactions. The research aims at selecting the peptide sequence that offers the best performance in terms of forming organized nanostructures for biotechnological applications (biosensing, tissue engineering, ...). In this field I have multiple ongoing collaborations with the Fukuda Group (Yokohama University, Japan), the group of Pierangelo Metrangola (Politecnico di Milano), and the group of Alessandro Gori (National Research Council of Italy). This is a topic of great relevance in the field of smart biomaterials, where molecular modeling can

provide significant insights towards the development of new materials. This research has been funded by CARIPLO foundation (Local PI) and by the Italian Minister of Foreign Affair (PI). In the field of biomaterial design I have published 6 peer-reviewed papers.

Relevant Collaborations

- Dr. Parisini, Italian Institute of Technology, Italy
Topic: Enzyme engineering
- Prof. Snedeker, ETH Zurich, Switzerland
Topic: Effect of age-induced glycation on collagen mechanics
- Prof. Buehler, Massachusetts Institute of Technology, USA
Topic: Multi-scale modeling of collagen
- Prof. Keating, Massachusetts Institute of Technology, USA
Topic: Design of protein binding peptides
- Prof. Metrangolo, Politecnico di Milano, Italy
Topic: Modelling of halogenated biomolecules
- Dr. Salmona, Istituto di Ricerche Farmacologiche “Mario Negri”, Italy
Topic: Modelling of amyloid proteins and anti-amyloidogenic drugs
- Dr. Gori, National Research Council, Italy
Topic: Design of self-assembling peptides
- Prof. Fleishman, Weizmann Institute of Science, Israel
Topic: In silico protein design
- Prof. Candiani, Politecnico di Milano, Italy
Topic: rational design of gene delivery vectors

Grants & Fellowships

Pending	“Misura per contrastare l’emergenza COVID-19 e altre emergenze virali del futuro” research grant from CARIPLO Foundation (PI)
Pending	H2020-MSCA-ITN-2020 “REDzyme: Rational Engineering and Design of enzymes” (Coordinator)
2019	Seed Funds from MIT International Science and Technology Initiatives (Co-PI, funding: 13k €)
2016	“Biomedical research conducted by young researchers” research grant from CARIPLO Foundation (PI, Grant ID 2016-0481, funding: 245k €)
2013	“International Short Visits” fellowship from Swiss National Science Foundation (Recipient, funding: 8k €).
2013	“Italy-Japan Scientific and Technological Cooperation Agreement” research grant from Italian Ministry of Foreign Affair (Principal Investigator, Grant ID JP13MO5, funding: 6k €)
2013	“Advanced Materials” research grant from CARIPLO Foundation (Local PI, Grant ID 2013-0766, funding: 330k €)
2010	“5 per mille Junior” research grant from Politecnico di Milano, Italy (Participant, funding: 68k€)
2010	MIT-Italy “Progetto Rocca” Postdoctoral fellowship (Recipient, funding: 32k €)
2007	Seed funds from MIT-Italy program “Progetto Rocca” (Participant, funding: 10k €)

Awards and Honors

<i>Pending</i>	Italian National Scientific Habilitation as Associate Professor in track 03/B2 (Principles of Chemistry for Applied Technologies)
10/2018	Italian National Scientific Habilitation as Full Professor in track 09/G2 (Bioengineering)
03/2017	Italian National Scientific Habilitation as Associate Professor in track 09/G2 (Bioengineering)
04/2017	Italian National Scientific Habilitation as Associate Professor in track 02/D1 (Applied Physics, Teaching and History of Physics)
2006	National Award from the Italian Bioengineering National Group (GNB) for the original and innovative Master Thesis in the field of Bioengineering.

Teaching Experience

2019-present	Responsible of the course <i>Industrial Project</i> (5 ECTS) (Bachelor Degree in Biomedical Engineering, Politecnico di Milano, Italy)
2019	Invited lecturer, Summer School “ <i>Intrinsically disordered proteins (IDPs) - From physical chemistry to pathogenic mechanisms</i> ”, 23-27 September 2019, Como (Italy). (2h)
2017-2019	Teaching assistant (40h/year) for the course <i>Biomechanics</i> (12 ECTS) (Bachelor Degree in Biomedical Engineering, Politecnico di Milano, Italy)
2017-2019	Teaching assistant (20h/year) for the course <i>Industrial Project</i> (5 ECTS) (Bachelor Degree in Biomedical Engineering, Politecnico di Milano, Italy)
2013-2019	Teaching for the biennial Doctoral Course "Simulation of molecular systems for chemistry, materials and biology" (PhD School of Politecnico di Milano) (8 h /edition)
2009-2015	Teaching assistant (50 h/year) for the course <i>Biomolecular Modelling Laboratory</i> (5 ECTS) (Master Degree in Biomedical Engineering, Politecnico di Milano, Italy)
2010-2015	Teaching assistant (8h/year) for the course <i>Cellular Bioengineering</i> (10 ECTS) (Master Degree in Biomedical Engineering, Politecnico di Milano, Italy)
July 2012	Invited lecturer for the Summer School “ <i>Materiomics: Multiscale Mechanics of Biological Materials and Structure</i> ”, at the Centre International des Sciences Mecaniques, Udine, Italy. (8h)

Students supervised

2009 – 2019	Supervision of 3 PhD student, 19 Master students (Dept. of Bioengineering, PoliMi, Italy), 1 Master student (ETH Zürich)
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After graduation, several of the 19 Master students supervised started a PhD (at EPFL, Switzerland; ETH Zürich, Switzerland; PoliMi, Italy; University of Fribourg, Switzerland; University of Brighton, UK; Universitat Pompeu Fabra, Spain).

Synthetic track record (as of April 2020, source: ISI Web of Science)

H-index: 19

Total number of peer-reviewed publications: 39

Citation count: 1459

Peer Reviewed Publications

1. **A. Gautieri**, M. Beeg, M. Gobbi, F. Rigoldi, L. Colomb, M. Salmona. 2019. *The Anti-Amyloidogenic Action of Doxycycline: A Molecular Dynamics Study on the Interaction with A β 42*. International Journal of Molecular Sciences 20, 4641. doi: 10.3390/ijms20184641.
2. **A. Gautieri**, A. Milani, A. Pizzi, F. Rigoldi, A. Redaelli, P. Metrangolo. 2019. *Molecular dynamics investigation of halogenated amyloidogenic peptides*. Journal of Molecular Modelling 25:124. doi:10.1007/s00894-019-4012-9
3. F. Rigoldi, S. Donini, F. Giacomina, F. Sorana, A. Redaelli, T. Bandiera, E. Parisini, **A. Gautieri**. 2018. *Thermal stabilization of the deglycating enzyme Amadoriase I by rational design*. Scientific Reports 8, article number 3042.
4. F. Rigoldi, S. Donini, A. Redaelli, E. Parisini, **A. Gautieri**. 2018. *Engineering of Thermostable Enzymes for Industrial applications*. APL Bioengineering 2, article number 011501 (**cover paper**).
5. E. Bianchi, M. Piergiovanni, C. Arrigoni, J. Fukuda, **A. Gautieri**, M. Moretti, G. Dubini. 2017. *Herringbone-like hydrodynamic structures in microchannels: A CFD model to evaluate the enhancement of surface binding*. Medical Engineering and Physics 48, 62-67.
6. F. Rigoldi, P. Metrangolo, A. Redaelli, **A. Gautieri**. 2017. *Nanostructure and stability of calcitonin amyloids*. Journal of Biological Chemistry 292, 7348-7357.
7. J. Enomoto, T. Kageyama, T. Osaki, F. Bonalumi, F. Marchese, **A. Gautieri**, E. Bianchi, G. Dubini, C. Arrigoni, M. Moretti, J. Fukuda. 2017. *Catch-and-Release of Target Cells Using Aptamer-Conjugated Electroactive Zwitterionic Oligopeptide SAM*. 2017. Scientific Report 7:43375.
8. **A. Gautieri**, F. Passini, M. Guizar-Sicairos, G. Carimati, P. Volpi, M. Moretti, A. Redaelli, M. Berli, J.G. Snedeker. 2016. *Advanced glycation end-products: mechanics of aged collagen from molecule to tissue*. Matrix Biology 59, 95-108.
9. A. Apicella, M. Marascio, V. Colangelo, M. Soncini, **A. Gautieri**, C.J.G. Plummer. 2016. *Molecular Dynamics Simulations of the Intrinsically Disordered Protein Amelogenin*. Journal of Biomolecular Structure and Dynamics 35, 1813-1823.
10. F. Rigoldi, L. Spero, A. Dalle Vedove, A. Redaelli, E. Parisini, **A. Gautieri**. 2016. *Molecular dynamics simulations provide insights into substrate specificity of FAOX family members*. Molecular Biosystems 12, 2622-2633.
11. F. Rigoldi, **A. Gautieri**, A. Dalle Vedove, A. Luccarelli, S. Vesentini, E. Parisini. 2016. *Crystal Structure of the Deglycating Enzyme Amadoriase I in its Free Form and Substrate-bound Complex*. Proteins: Structure, Function and Bioinformatics 84, 744-758 (**cover paper**).
12. JG Snedeker, **A. Gautieri**. 2014. *The role of collagen crosslinks in ageing and diabetes - the good, the bad, and the ugly*. Muscles, Ligaments and Tendons Journal 4, 303-308
13. L. Russo, A. Sgambato, P. Giannoni, R. Quarto, S. Vesentini, **A. Gautieri**, A., L. Cipolla. 2014. *Response of osteoblast-like MG63 on neoglycosylated collagen matrices*. Medchemcomm 5, 1208-1212.
14. A.K Nair, **A. Gautieri**, M.J. Buehler. 2014. *Role of Intrafibrillar Collagen Mineralization in Defining the Compressive Properties of Nascent Bone*. Biomacromolecules 15, 2494-2500.
15. L. Russo, **A. Gautieri**, M. Raspanti, F. Taraballi, F. Nicotra, S. Vesentini, L. Cipolla. 2014. *Carbohydrate-functionalized collagen matrices: design and characterization of a novel neoglycosylated biomaterial*. Carbohydrate Research 389, 12-17.
16. **A. Gautieri**, A. Redaelli, M.J. Buehler, S. Vesentini. 2014. *Age- and diabetes-related nonenzymatic crosslinks in collagen fibrils: Candidate amino acids involved in Advanced Glycation End-products*. Matrix Biology 34, 89-95.
17. G. S. Ugolini, **A. Gautieri**, A. Redaelli, M. Soncini. 2013. *Structural analysis and ion translocation mechanisms of the muscle-type acetylcholine receptor channel*. Journal of applied biomaterials & functional materials 11, 53-60.
18. A.K. Nair, **A. Gautieri**, S.W. Chang and M.J. Buehler. 2013. *Molecular mechanics of mineralized collagen fibrils in bone*. Nature Communications 4, 1724.
19. **A. Gautieri**, S. Vesentini, A. Redaelli and R. Ballarini. 2013. *Modeling and measuring visco-elastic properties: from collagen molecules to collagen fibrils*. International Journal of Non-linear Mechanics 56, 25-33.
20. S. Vesentini, A. Redaelli, **A. Gautieri**. 2013. *Nanomechanics of collagen microfibrils*. Muscle, Ligament and Tendon Journal 3, 23-34.

21. **A. Gautieri**, M.I. Pate, S. Vesentini, A. Redaelli, M.J. Buehler. 2012. *Hydration and distance dependence of intermolecular shearing between collagen molecules in a model microfibril*. J. Biomechanics 45, 2079-2083.
22. **A. Gautieri**, S. Vesentini, A. Redaelli, M.J. Buehler. 2012. *Osteogenesis imperfecta mutations lead to local tropocollagen unfolding and disruption of H-bond network*. RCS Advances 2, 3890-3896.
23. Z. Qin, **A. Gautieri**, A.K. Nair, H. Inbar and Markus J. Buehler. 2012. *Thickness of hydroxyapatite nanocrystal controls mechanical properties of the collagen-hydroxyapatite interface*. Langmuir 28, 1982-1992.
24. **A. Gautieri**, S. Vesentini, A. Redaelli, M.J. Buehler. 2012. *Viscoelastic properties of model segments of collagen molecules*. Matrix Biology 31, 141-149.
25. **A. Gautieri**, A. Mezzanzanica, A. Motta, S. Vesentini, A. Redaelli. 2012. *Atomistic modeling of water diffusion in hydrolytic biomaterials*. Journal of Molecular Modeling 18, 1495-501.
26. **A. Gautieri**, S. Vesentini, A. Redaelli, M.J. Buehler. 2011. *Hierarchical Structure and Nanomechanics of Collagen Microfibrils from the Atomistic Scale Up*. Nano Letters 11, 757-66.
27. M. Srinivasan, S.G.M. Uzel, **A. Gautieri**, S. Keten, M.J. Buehler. 2010. *Linking Genetics and Mechanics in Structural Protein Materials: A Case Study of an Alport Syndrome Mutation in Tropocollagen*. Mathematics and Mechanics of Solids 15, 755-770.
28. **A. Gautieri**, A. Russo, S. Vesentini, A. Redaelli, M.J. Buehler. 2010. *Coarse-Grained Model of Collagen Molecules Using an Extended MARTINI Force Field*. Journal of Chemical Theory and Computation 6, 1210-1218.
29. **A. Gautieri**, S. Vesentini, A. Redaelli. 2010. *How to predict diffusion of medium-sized molecules in polymer matrices. From atomistic to coarse grain simulations*. Journal of Molecular Modeling 16, 1845-1851.
30. **A. Gautieri**, M. Ionita, D. Silvestri, E. Votta, S. Vesentini, G.B. Fiore, N. Barbani, G. Ciardelli, A. Redaelli. 2010. *Computer-Aided Molecular Modeling and experimental validation of water permeability properties biosynthetic materials*. Journal of Computational and Theoretical Nanoscience 7, 1287-1293.
31. Srinivasan, M., Uzel, S.G.M., **Gautieri, A.**, Keten, S. and Buehler, M.J. 2009. *Alport Syndrome mutations in type IV tropocollagen alter molecular structure and nanomechanical properties*. Journal of Structural Biology 168, 503-510.
32. **A. Gautieri**, Uzel S., Vesentini S., Redaelli A., and Buehler M.J. 2009. *Molecular and mesoscale mechanisms of Osteogenesis Imperfecta disease in collagen fibrils*. Biophysical Journal 97, 857-865.
33. **A. Gautieri**, Buehler, M. J., and Redaelli, A. 2009. *Deformation rate controls elasticity and unfolding pathway of single tropocollagen molecules*. Journal of the Mechanical Behavior of Biomedical Materials, 2, 130-137.
34. **A. Gautieri**, Vesentini S., Redaelli A., and Buehler M.J. 2009. *Intermolecular slip mechanism in tropocollagen nanofibrils*. International Journal of Materials Research, 100(7), pages 921-924.
35. **A. Gautieri**, S. Vesentini, A. Redaelli, M.J. Buehler. 2009. *Single molecule effects of Osteogenesis Imperfecta*. Protein Science 18, 161-168.

Books & Book Chapters

1. **A. Gautieri**, M.J. Buehler. *Multiscale modeling of biomaterials and tissues*. In "Materiomics: Multiscale Mechanics of Biological Materials and Structures", R. Ballarini and M. Buehler (Editors). Springer Edition, 2013. ISBN 978-3-7091-1573-2.
2. P. Zunino, S. Vesentini, A. Porpora, J.S. Soares, **A. Gautieri**, A. Redaelli. *Multiscale computational analysis of degradable polymers*. In "Modelling Physiological Flows", D. Ambrosi, A. Quarteroni, G. Rozza (Editors). Springer Edition, 2010. ISBN 978-88-470-1935-5
3. A. Redaelli, M. Soncini, S. Vesentini, E. Votta, M.A. Deriu, **A. Gautieri**, G.B. Fiore, F.M. Montevercchi, S.Enemark, I.Aprodu and M.Ionita. *Multiscale modelling in biomechanical applications*. In "The Nanomechanics in Italy", Ed. Research Signpost, 2007. ISBN: 978-81-308-0237-4.

Oral Presentations at International Conferences

1. **A. Gautieri**, F. Rigoldi, A. Dalle Vedove, A.P. Lucarelli, S. Vesentini, E. Parisini. *Collagen glycation and deglycation. Candidate locations of collagen non-enzymatic glycation and characterization of an Amadoriase enzyme for its prevention*. 40TH Federation of European Biochemical Society Congress, 4-9 July 2015, Berlin, Germany.
2. **A. Gautieri**, L. Bernardi, F. Crippa, S. Vesentini, J.G. Snedeker. *Collageing: understanding age- and diabetes-related glycation in connective tissues*. World Congress of Biomechanics 2014, 6-13 July, Boston, USA.
3. **A. Gautieri**, A. Nair, S. Vesentini, M.J. Buehler. *Towards atomistic modeling of bone. Investigation of the collagen-mineral interface and of the mineralized collagen fibrils mechanics*. World Congress of Computational Mechanics 2012, 8-13 July, Sao Polo, Brasil.
4. **A. Gautieri**, S. Vesentini, A. Redaelli and M.J. Buehler. *Atomistic and Coarse-Grain Modeling of a Collagen Type I Fibril*. Engineering Mechanics Institute 2011, June 2-4, 2011, Boston, MA, USA.
5. **A. Gautieri**, S. Vesentini, A. Redaelli and M.J. Buehler. *Computational multiscale studies of collagen tissues in the context of brittle bone disease osteogenesis imperfecta*. Material Research Society Spring Meeting 2010, April 5-9, San Francisco, California, USA.
6. **A. Gautieri**, S. Vesentini, A. Redaelli. *Predicting water diffusivity in biodegradable materials. An atomistic simulation approach*. Computer Methods in Biomechanics and Biomedical Engineering 2010, February 24-27, Valencia, Spain.
7. **A. Gautieri**, S. Uzel, S. Vesentini, A. Redaelli and M.J. Buehler. *Molecular and mesoscale mechanisms of Osteogenesis Imperfecta disease in collagen fibrils*. ASME Summer Bioengineering Congress 2009, June 20-24, Lake Tahoe, California, USA.
8. **A. Gautieri**, M. Srinivasan, S. Keten and M.J. Buehler. *Osteogenesis Imperfecta Mutations in Tropocollagen Protein Domains Lead to Molecular Softening and Reduced Intermolecular Adhesion*. Material Research Society Spring Meeting 2009, April 13-17, San Francisco, California, USA.
9. **A. Gautieri**, M. J. Buehler, A. Redaelli. *Pulling rate dependence of the nanomechanics of single tropocollagen molecules*. Proceedings of the World Congress Computational Mechanics 2008. June 30-July 04, 2008, Venice, Italy.

Patents

A. Gautieri, E. Parisini, F. Rigoldi, S. Donini, A. Redaelli. 2017. *Thermostabilized Amadoriases And Uses Thereof*. Patent n° PCT/IB2018/054582, filed June 23rd, 2017.

Outreach activities

2019	The BioMolEng Lab participated to the MeetMeTonight@Milan event (European Researchers' Night)
2018-2019	Outreach activity for high school students (one week training activity in the lab) within the School@DEIB framework.
2018	Open Lab activity focused on Protein Folding for the "STEM in the City" event organized by the City of Milan.

Other

2017- current	Volunteering as Mountaineering instructor at Club Alpino Italiano (Corsico, MI)
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Data

29/4/2020

Luogo

Milano