

Curriculum Vitae Matteo Ceccarelli

Citizen: Italian

Mother Tongue: Italian

Other Languages: English and French

Total number of Articles: 120 (Research Gate), 98 (SCOPUS)

Total citation: 3871 (Research Gate), 2230 (SCOPUS)

H-factor: 36 (Research Gate), 33 (SCOPUS)

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SCOPUS-ID: 7102783662

Research-ID: C-8557-2018

EDUCATION:

- 2013: Habilitation as Full Professor in Applied Physics
- 2010: Habilitation as Associate Professor in Applied Physics
- 1997-May 2001: PhD at the École Normale Supérieure, Lyon, France: *Numerical simulations of the primary electron transfer in a photosynthetic reaction center*
Advisors: Prof. S. Baroni, International School for Advanced Study SISSA/ISAS, Trieste IT and Dr. M. Marchi, Commissariat à l'Énergie Atomique CEA, Saclay FR.
- 1988-1994: Laurea in Physics, Università degli Studi di Cagliari, Italy: *Numerical methods for simulating macromolecular systems*
Advisors: Prof. F. Meloni, Università degli Studi di Cagliari (IT) and Prof. S. Baroni, SISSA/ISAS, Trieste (IT)

CURRENT POSITIONS

2022 – Full Professor, Department of Physics, University of Cagliari, Italy

2018 – Associate Researcher, Istituto Officina dei Materiali (IOM), CNR, Italy

PREVIOUS POSITIONS

2011 – 2022 Associate Professor, Department of Physics, University of Cagliari, Italy

2004 – 2011 Assistant Professor, Faculty of Medicine and Surgery, University of Cagliari, Italy

2001 – 2004 Postdoctoral Researcher, ETHZ/Parrinello Group, Lugano, Switzerland

2001 – 2001 Postdoctoral Researcher, MPI/Parrinello Group, Stuttgart, Germany

1998 – 2001 Researcher, Ecole Normale Supérieure de Lyon, Lyon, France

1997 – 1998 Stage at Cecam/ENS Lyon (FR) within the INFM program “Progetto Sud”

1996 – 1997 Software Engineering, Techso and StMicroelectronics, Cagliari, Italy

1995 – 1996 Stage at CEA-Saclay on Biophysics (FR)

1995 Stage at CNR/Università degli Studi di Cagliari (IT)

1994 Stage at SISSA/ISAS Trieste (IT)

PROFESSIONAL EXPERIENCES

2022 Consultant for Basilea Pharmaceutica (CH) on permeation of antibiotics in Gram negative Bacteria

2018 Consultant for VenatorX (US) on permeation of antibiotics in Gram negative Bacteria

2010 Consultant for Johnson&Johnson (US) on permeation of antibiotics in Gram negative Bacteria

RESUME

He received in 2001 the PhD in Biophysics from ENS Lyon as Marie Curie Fellow at CECAM and then he performed research on computational methods tailored for biophysical systems at MPI-Stuttgart and ETH-Zurich, under the supervision of Prof. Parrinello. Since 2004 he is appointed at the University of Cagliari.

He is an expert of transport phenomena at the molecular scale, passive diffusion through nanopores, porins and ion channels (from prokaryotic and eukaryotic cells) and active diffusion within receptors and transporters; characterization of peptides and other small-molecules in solution; force field development for small molecules; ligand-protein interactions, and computational methods for enhanced sampling.

He was local coordinator of two ITN projects for the part dedicated to modelling and was coordinator of a Marie Curie project for a post-doc (AQPAssoc). He was one of the three promoter of the IMI project

“Translocation”, thus part of its scientific committee and appointed as academic leader of the WP dedicated to transport properties through porins, the most important topic with 7.5 Meuro budget (over 15 Meuro in total for 8 WPs) and 7 participating groups, and strongly involved in the WP dedicated to receptors and active transporters for pursuing the Trojan Horse approach. Thanks to these experiences he has acquired a very deep and extensive knowledge of passive diffusion of antibiotics through bacterial porins. He has been consultant of a few pharmaceutical companies with the aim to explicitly enhance permeation for lead antibiotics in early drug discovery, an approach that never was used in the past.

TRANSVERSAL SKILLS

He has a long experience with the management of European projects and in 2007 he was appointed by its department to follow a semester of coaching/training as Project Manager, organized by the Italian CRUI. He has worked in contact with many important computer centers in Europe (Cea/Grenoble and Idris/Paris, CSCS/Manno, Cineca/Bologna, Caspur/Roma and Cybersar/Cagliari).

TEACHING ACTIVITIES

He provides lectures of General Physics at the Faculty of Medicine and Surgery. Since 2018 he has a course in Biophysics at the Faculty of Sciences. He is constantly in contact with a biological-medical environment, also through the participation to Specialization Schools of Medicine (Medical Physics, Anaesthesia and Reanimation, Orthopaedic).

INSTITUTIONAL RESPONSIBILITIES

- 2021 – Chairman of the Joint Teaching Staff/Student Committee at the Faculty of Medicine and Surgery, University of Cagliari, Italy
- 2018 – 2021 Coordinator of the Master in Health Professions of (Diagnostic) Technical Sciences, University of Cagliari, Italy
- 2017 – Responsible of the Bachelor’s degree in Imaging and Radiotherapy Techniques, University of Cagliari, Italy
- 2015 – 2021 Faculty member, Faculty of Medicine and Surgery, University of Cagliari, Italy
- 2015 – 2017 Coordinator of the Bachelor’s degree in Biomedical Laboratory Techniques, University of Cagliari, Italy
- 2012 – Member of the Medical School in Medical Physics, University of Cagliari, Italy
- 2010 – 2015 Member of Scientific Board IOM/CNR, Italy
- 2006 – Member of the PhD School in Physical Sciences, University of Cagliari, Italy

MAJOR COLLABORATIONS

- Prof. Mathias Winterhalter, *Single-molecule/single-channel electrophysiology on nanopores*, Jacobs University, Bremen
- Dr. Jean-Marie Pagès, *Permeation of molecules through porins and accumulation in Gram negative bacteria*, Aix-Marseille University, INSERM, IRBA, MCT, Marseille
- Prof. James H. Naismith and Dr. Lucile Moynié, *Structural Characterisation of bacterial porins and transporters*, Division of Structural Biology, Wellcome Trust Centre of Human Genomics & The Research Complex at Harwell & The Rosalind Franklin Institute, Oxford
- Prof. Lucija Peterlin Mašič, *Optimization of antinfectives for enhanced permeation in Gram negative bacteria*, Faculty of Pharmacy, University of Ljubljana, Slovenija
- Prof. Daniel Borgis, *Transport of small molecules, ligands, gases*, ENS-Chimie Paris

EUROPEAN/INTERNATIONAL PROJECTS:

- 2019-2021 JPI-EC-AMR, Reset-Me, External Partner
- 2013-2018 IMI project, ND4BB platform on antibiotics, Academic Leader of WP2
- 2013-2016 FP7-ITN on antibiotics permeation, Local Coordinator
- 2010-2012 FP7-IIF, aquaporin channels, Coordinator
- 2006-2009 FP6-RTN on antibiotics permeation, Local Coordinator
- 2002-2003 Top-Nano21, Molecular Switches, Switzerland

NATIONAL PROJECTS

INF-ACT PE00000007 2022 (Emerging Infectious Diseases, PNRR)
PRIN 2022 (Porins-Enzymes interactions), PRIN 2015 (Intracellular channels), 2013 (Eukaryotic porins),
2007 (Hemoglobins)
2008-2009 INFM/CNR Seed projects for young researchers (Globins)

REGIONAL PROJECTS

2020-2022 Fondazione Banco di Sardegna, Analysis of bacterial envelopes, the S-layer
2017-2019 Fondazione Banco di Sardegna, Physical Chemistry of Proteins in solutions
2010, 2011 2012, 2014, 2016: LR7
2010-2011 LR7, Inhibitors for Gram positive cocci
2006-2008 MIUR, program in biomedical applications, Antiviral Compounds
2006-2008 Project Cybersar

RECENT ORAL CONTRIBUTIONS

- CECAM workshop, Lausanne 2022
- Frontiers in ion channels and nanopores: theory, experiments and simulations, online, 2021
- *SIF-2020*, online
- Processes in Isotopes and Molecules 2019, Cluj-Napoca (RO)
- SIF-2019, L'Aquila, *Invited*
- CECAM Conference 50 years, Lausanne
- CECAM workshop: *Network Analysis*, Lyon 2019
- ACS FALL 2019, San Diego (US)
- ECCMID 2019, Amsterdam
- National Conference SIBPA: Ancona 9-2018
- Workshop: *Nanofluidics in Physics and Biology*, 2018 Lyon (FR)
- Workshop: *Getting small drug-like molecules into Gram- bacteria*, 2018 Oxford (UK)
- School on Biophysics: SIBPA, Venice 2018 (IT)

VISITS FOR TEACHING/RESEARCH

- ENS-Chimie, 3-4/2022, Paris (FR)
- King's College 3/2017, PhD school in Nonlinear Phenomena, London (UK)
- DAAD/Jacobs University Bremen 3-4/2010, Master in Biology, Bremen (DE)

SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS

2004 – 9 Postdocs, 8 PhD, 11 Master Student, 3 Graduate Students

NATIONAL/INTERNATIONAL PRIZE AWARDS

- 1998: PhD Marie Curie Fellow at ENS-Lyon (FR)
- 2008: CNR Seed grant for young researchers
- 2012: Second best presentation in Physics, National Meeting SIF, L'Aquila (IT)
- 2019: Best poster presentation, Novel Antimicrobial and AMR Diagnostic 2019, Berlin

ORGANISATION OF SCIENTIFIC MEETINGS

- 2023 CECAM Workshop, *Nanofluidics in physics and biology*, 40 participants, Lyon, France
- 2021 CECAM Workshop, *Nanopore Translocation and Nanochannel Confined Biopolymers*, 40 participants, Trieste, Italy
- 2017 Final Meeting project MSCA, 30 participants, Germany
- 2015 EU-ETN Workshop, *Drug Discovery*, 50 participants, Italy
- 2009 CECAM & ESF Workshop, *From Structure to Function: Influx and Efflux Systems*, 50 participants, Italy
- 2006 Workshop for Laurea ad Honorem to Prof Michele Parrinello, *Simulations and rare events*, 30 participants, Italy

REVIEWING ACTIVITIES

- Projects: Italy (PRIN, Rita Levi Montalcini, EUROSTAR), France (ANR), Poland (Narodowe Centrum Nauki), Germany (DAAD), EU (JPIAMR, COST), Denmark (DFF)

- PhD Examiner: SISSA (IT), IIT (India), Cardiff Univ. (UK), Jacobs Univ. (DE)
- Tenure Track Positions (Univ. Modena e Reggio, Univ. of Firenze)
- HPC Projects: PRACE Tier-0, CINECA TIER-1
- Nature group journals, American Chemical Society journals, Royal Society of Chemistry journals, BBA journals, Plos journals
- Editorial Board Member: *Antibiotics* (ISSN 2079-6382), MDPI, Switzerland

5 SELECTED PUBLICATIONS

1. J. Vergalli, I.V. Bodrenko, M. Masi, L. Moynié, S. Acosta-Gutierrez, J.H. Naismith, A. Davin-Régli, **M. Ceccarelli**, B. v d Berg, M. Winterhalter, & J.-M. Pagès, “*Porins and small-molecule translocation across the outer membrane of Gram-negative bacteria*” *Nat Rev Micro* 33, 1831–13 (2020).
2. L. Moynié, S. Milenkovic, G. L A Mislin, V. Gasser, G. Mallocci, E. Baco, R. P McCaughan, M. G P Page, I. J Schalk, **M. Ceccarelli**, & J. H Naismith “*The complex of ferric-enterobactin with its transporter from Pseudomonas aeruginosa suggests a two-site model*” *Nat. Comm.* 10, 3673 (2019).
3. S. Acosta-Gutierrez, L. Ferrara, M. Pathania, M. Masi, J. Wang, I. V Bodrenko, M. Zahn, M. Winterhalter, R. A Stavenger, J.-M Pagès, J. H Naismith, B. van den Berg, M. G P Page, & **M. Ceccarelli** “*Getting Drugs into Gram-Negative Bacteria: Rational Rules for Permeation through General Porins*” *ACS Infect. Dis.* 4, 1487–1498 (2018).
4. H. Bajaj, S. Acosta-Gutierrez, I. V Bodrenko, G. Mallocci, M. A Scorciapino, M. Winterhalter, & **M. Ceccarelli** “*Bacterial Outer Membrane Porins as Electrostatic Nanosieves: Exploring Transport Rules of Small Polar Molecules*” *ACS Nano* 11, 5465–5473 (2017).
5. Scorciapino, M. A., Robertazzi, A., Casu, M., Ruggerone, P. & **Ceccarelli, M.** “Heme Proteins: The Role of Solvent in the Dynamics of Gates and Portals.” **132**, 5156–5163 (2010).