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Personal

Date of birth	March 27, 1982
Place of birth	Trescore Balneario (BG), Italy

Academic Appointments

01/2017 -	Assistant Researcher, Princeton University, USA PI: Prof. Roberto Car Research: Realization and development of the <i>GeM</i> (Geometry Matching) algorithm Characterization of water properties in biological environments Hyperuniformity and large-scale structures in disordered media Statistical physics of continuous random networks
01/2013 - 12/2016	Post doctoral Associate in Theoretical Chemical Physics, Princeton University, USA PI: Prof. Roberto Car Research: Realization and development of the <i>GeM</i> (Geometry Matching) algorithm Water and ice under extreme thermodynamic conditions Role of many body interactions in water and molecular crystals Statistical physics of continuous random networks Analytical number theory
02/2011 - 12/2012	Post doctoral Scholar in Theoretical Chemical Physics, Centre National de la Recherche Scientifique (CNRS), Paris, France PI: Dr. Riccardo Spezia Research: New models to understand the role of the dielectric friction in liquids Development of new classical force fields to study actinides in water Development of new classical force fields to study complexation of lanthanoids with carbonate ions

Education

12/2007 - 12/2010	Ph.D. , University of Milan (Italy) / École normale supérieure of Paris (France) Title: "Wave packets approaches to dissipative quantum dynamics"
09/2005 - 10/2007	MSc <i>cum laude</i> , University of Milan (Italy) Title: "About the behaviour of kinetic constants for the radiative association reactions in the limit of $T \rightarrow 0$ K"

Publications

- 1 **F. Martelli**, S. Torquato, N. Giovanbattista and R. Car
"Large-scale structure and hyperuniformity in amorphous ices",
Submitted to Physical Review Letters
- 2 **F. Martelli**, S. Torquato, N. Giovanbattista, H.-Y. Ko and R. Car
"Short- and intermediate-range order in amorphous ices",
Submitted to Frontiers of Physics
- 3 **F. Martelli**, H.-Y. Ko, C. Calero Borallo and G. Franzese
"Structural properties of water confined by phospholipid membranes",
arXiv:1703.07835 [cond-mat.soft], *Submitted to Frontiers of Physics*
- 4 J. C. Palmer, A. Haji-Akbari, R. S. Singh, **F. Martelli**, R. Car, A. Z. Panagiotopoulos and P. G. Debenedetti
"Comment on: The Putative Liquid-Liquid Transition is a Liquid-Solid Transition in Atomistic Models of Water [Parts I and II: J. Chem. Phys. 135, 134503 (2011); J. Chem. Phys. 138, 214504 (2013)]"
Submitted to Journal of Chemical Physics
- 5 **F. Martelli**, H.-Y. Ko, E. C. Oğuz and R. Car
"A local order metric for condensed phase environments",
<http://arxiv.org/abs/1609.03123>, under review at *Physical Review B*
- 6 J. C. Palmer, **F. Martelli**, Y. Liu, R. Car, Z. Panagiotopoulos and P. Debenedetti
"Metastability and not criticality Reply"
Nature, **531**, E2-E3 (2016)
- 7 J. C. Palmer, R. S. Singh, R. Chen, **F. Martelli** and P. G. Debenedetti
"Density and bond-orientational relaxations in supercooled water"
Molecular Physics, **114**, 2580 (2016)
- 8 B. Santra, R. DiStasio Jr., **F. Martelli** and R. Car
"Local Structure Analysis of *Ab Initio* Liquid Water",
Molecular Physics, **113**, 2829 (2015)
- 9 J. C. Palmer, **F. Martelli**, Y. Liu, R. Car, Z. Panagiotopoulos and P. Debenedetti
"Metastable liquid-liquid transition in a molecular model of water"
Nature, **510**, 7505 (2014)
Shared cover Article
Highlighted in Nature Physics (N&V by F. W. Starr)
Highlighted in Nature Materials (N&V by C. A. Angell)
- 10 **F. Martelli**, R. Vuilleumier, Y. Jeanvoine, T. Vercoeur and R. Spezia
"Hydration properties of Lanthanoid(III) carbonate complexes in liquid water by molecular dynamics simulations"
Physical Chemistry Chemical Physics, **16**, 3693 (2014)
- 11 **F. Martelli**, S. Abadie, J.-P. Simonin, R. Vuilleumier and R. Spezia
"Lanthanoids(III) and actinoids(III) in water: diffusion coefficients and hydration enthalpies from polarizable molecular dynamics simulations"
Pure and Applied Chemistry **85**, 237 (2013)
- 12 P. D' Angelo, **F. Martelli**, R. Spezia, A. Filipponi and M. A. Denecke
"Hydration properties and ionic radii of actinide(III) in aqueous solutions",
Inorganic Chemistry, **52**, 10318 (2013)
- 13 **F. Martelli**
"Dealing with prime numbers I.: On the Goldbach conjecture",
arXiv:1309.5895 [math.NT], (2013)
- 14 **F. Martelli**, R. Vuilleumier, J.-P. Simonin and R. Spezia
"Varying the charge of small cations in liquid water: Structural, transport and thermodynamic properties",
Journal of Chemical Physics **137**, 164501 (2012)
- 15 Y. Jeanvoine, P. Miró, **F. Martelli**, C. J. Cramer, R. Spezia
"Electronic structure and Bonding of Lanthanoid(III) Carbonates",
Physical Chemistry Chemical Physics, **14**, 14822 (2012)

- 16 M. Duvail, **F. Martelli**, P. Vitorge, and R. Spezia
 "Polarizable interaction potential for molecular dynamics simulations of actinoids(III) in liquid water"
Journal of Chemical Physics **135**, 044503 (2011)
- 17 R. Martinazzo, K. H. Hughes, **F. Martelli**, and I. Burghardt
 "Effective spectral densities for system-environment dynamics at conical intersections: S₂-S₁ conical intersection in pyrazine"
Chemical Physics, **377**, 21-29 (2010)
Selected paper for the special issue "Dynamics at Conical Intersections", (2013)
- 18 R. Martinazzo, I. Burghardt, **F. Martelli**, and M. Nest
 "Local coherent-state approximation to system-bath quantum dynamics",
 in *Multidimensional Quantum Mechanics with Trajectories* Eds. D. V. Shalashilin and M. P. de Miranda (CCP6, Daresbury Laboratory, 2009), ISBN 978-0-9545289-8-0 (2009)
- 19 I. Burghardt, R. Martinazzo, **F. Martelli**, and G. A. Worth
 "The G-MCTDH method: correlated system-bath dynamics using Gaussian wave packets"
 in *Multidimensional Quantum Mechanics with Trajectories* Eds. D. V. Shalashilin and M. P. de Miranda (CCP6, Daresbury Laboratory, 2009), ISBN 978-0-9545289-8-0 (2009)

Oral communications

Invited talks

- 1 "A local order metric for condensed phase structures"
School on Water and Water Systems, Ettore Majorana Centre (Italy), July 28 2016
- 2 "The microscopic pathways of ice nucleation in supercooled conditions"
Seminar in Prof. Hartmut Löwen group, Institut for Theoretical Physics, University Heinrich-Heine, Düsseldorf (Germany), October 8th 2015
- 3 "The role of convex polyhedra in supercooled water and ice nucleation"
Seminar in Prof. Lars Pettersson's group, Department of Physics, Stockholm University, Stockholm (Sweden), October 5th 2015
- 4 "Understanding crystallization in deeply undercooled water"
FISMAT2015, University of Palermo, Palermo (Italy), October 1st 2015
- 5 "The role of convex polyhedra in ice nucleation"
PCTS Workshop "Water nucleation", Princeton Center for Theoretical Sciences, Princeton (USA) April 23-24 2015
- 6 "Structure and topology of supercooled water in the no man's land"
Seminar at CEA-ICSM site in Marcoule (France) September 2nd 2014
- 7 "Phase transitions in supercooled ST₂ water"
Seminar in Prof. Francesco Sciortino's group, Department of Physics, University "La Sapienza", Rome (Italy), August 26th 2013
- 8 "Polarizable model for ion hydration: an interplay between experiment and theory"
CECAM Workshop "Brainstorm meeting on the development of next generation force fields", University Pierre et Marie Curie, Paris (France), September 12th-14th 2011
- 9 "Modelling exciton transfer in dissipative media"
Seminar in Prof. Chantal Daniel's group, Department of Chemistry, University of Strasbourg, Strasbourg (France), September 30th 2010
- 10 "A model to study excitonic energy transfer: applications to α -helices"
JCM2010, University Pierre et Marie Curie, Paris (France), May 27th-28th 2010

Contributed talks

- 11 "Short-, Intermediate- and Long-range order in amorphous ices"
APS meeting 2017, New Orleans, LA, March 13-17 2016
- 12 "A new graph-matching-based algorithm to study dynamical processes"
APS meeting 2016, Baltimore, MD, March 14-18 2016
- 13 "Liquid-liquid coexistence and crystallization in supercooled ST₂ water"
EPS meeting Condensed Matter in Paris, Paris (France) August 24-29 2014
- 14 "Supercooled water: liquid-liquid coexistence and complex crystallization in the ST₂ model"
CECAM workshop WaterEurope, Zaragoza (Spain), June 12-14 2014
- 15 "Liquid-liquid coexistence and crystallization in supercooled ST₂ water"
APS meeting 2014, Denver, CO, March 3-7 2014
- 16 "Dynamics and complexation of lanthanoids and actinoids in aqueous solutions"
Journées Modélisation de l'Ens-ENSCP Paris (France), May 18th 2011
- 17 "Modelling exciton transfer in dissipative media"
XXXIX Congress of the Italian Chemical Society, Stresa (Italy), September 20th-24th 2010

Grants/Computer Allocations

- 2017 **NERSC Award of 3.424 M CPU Hours**
National Energy Research Scientific Computing Center and the U.S. Department of Energy (DOE)
Project: PBE+vdW pyridine polymorphic stability using variational free energy sampling technique
PI: H.-Y. Ko
Co-PI: **F. Martelli**, R. Car
- 2015 **ASCR Leadership Computing Challenge (ALCC) Award of 175 M CPU Hours**
Argonne National Laboratories and the U.S. Department of Energy (DOE)
Project: Anomalous Density Properties and Ion Solvation in Liquid Water: A PathIntegral *Ab Initio* Study
PI: R. A. DiStasio Jr.
CoPIs: **F. Martelli**, B. Santra, H.-Y. Ko, X. Wu, M. Ceriotti, A. Selloni, and R. Car
- 2015 **NERSC Award of 1 M CPU Hours**
National Energy Research Scientific Computing Center and the U.S. Department of Energy (DOE)
Project: Ions solvation under extreme conditions
PI: **F. Martelli**
Co-PI: R. Car
- 2014 **ASCR Leadership Computing Challenge (ALCC) Award of 350 M CPU Hours**
Argonne National Laboratories and the U.S. Department of Energy (DOE)
Project: Ion Solvation, Catalytic Interfaces, and Extreme Aqueous Environments: An *Ab Initio* Study of Liquid Water
PI: Robert A. DiStasio Jr.
Co-PIs: **F. Martelli**, D. Limmer, B. Santra, H.-Y. Ko, M. Cerriotti, A. Selloni, and R. Car

Awards/Fellowships

- 2008 **Vinci Project 2008 Financial Grant of 5000 Euro**
Italian-French University
Project: Wave Packet Approaches to Dissipative Quantum Dynamics
- 2007 **Italian Ministry of University and Research Financial Grant for a PhD position**

Teaching activities

2016	Princeton University (USA): Monte Carlo and Molecular Dynamics Simulation in Statistical Physics and Materials Science (PhD School)
2011 - 2012	University of Evry val d'Essonne (France): Quantum Mechanics and Structure of Matter (MSc class of Engineering)
2009 - 2010	University of Milan (Italy): Thermodynamics (BSc class in Applied and Environmental Chemistry)
2009 - 2010	University of Milan (Italy): Density Matrix Theory (MSc class in Theoretical Chemistry)

Teaching qualifications

2012	Teaching qualification from the French Ministry of Higher Education and Research to apply for Assistant Professorships in Theoretical and Physical Chemistry
2012	Teaching qualification from the French Ministry of Higher Education and Research to apply for Assistant Professorships in Physics of Fluids

Reviewing activities

2012 -	Physical Review Letters, Physical Review E
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Visiting positions

2007 - 2010	Theoretical Chemical Physics Group, École normale supérieure of Paris (France)
2009	Numerical Analysis Group, Department of Mathematics, University of Tübingen (Germany)

In the news

2015	"Chimico e matematico, qui libero di cercare" as featured in the Italian newspaper L'Eco di Bergamo
2014	"Familiar yet strange: Water's 'split personality' revealed by computer model" as featured in the magazines: Phys.org, ScienceDaily, ScienceNewline, R&D, EurekAlert, reOrbit, Hispanic Business (June, 18 2014)
2006	"Quattro bergamaschi nel club dei cervelloni" as featured in the Italian newspaper L'Eco di Bergamo

Outreach and non-scientific publications

2015	Scientific collaborator for the movie "Bad Vegan and the Teleportation Machine" Director: Anton Goenechea
2012-	Scientific reporting for the Italian newspaper "Il fatto quotidiano" Presentation of the latest scientific discoveries to the general public
2012	"Germogli", Webster Press, ISBN: 8889655208 Poems collection

Affiliations

2017 -	American Association for the Advancement of Science
2014 -	American Chemical Society
2013 -	American Physical Society