

Marina Macchiagodena

Personal information

Marina Macchiagodena
March, 23th 1982 Larino (CB), Italy
Italian nationality
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I have studied chemistry and subsequently I achieved my PhD for structural characterization of ionic liquids. At present, I am a postdoctoral researcher at Scuola Normale Superiore in Pisa. I have a strong aptitude to work in a multicultural environment and I am able to adapt to a variety of situations due to my work experiences in different groups and in different countries.

Professional Experience

20th April 2015 – present, Pisa, *Italy*

Postdoctoral Researcher

Scuola Normale Superiore
Research group led by Prof. Vincenzo Barone

Main subjects: Classical Molecular Dynamics, Structural Characterization, Force Fields development, Organic Solvents.

1st February 2013 – 31st May 2014, Bonn, *Germany*

Postdoctoral Researcher

Mulliken Center for Theoretical Chemistry, Institut für Physikalische und Theoretische Chemie
Rheinische Friedrich-Wilhelms-Universität
Research group led by Prof. Dr. Barbara Kirchner

Main subjects: Ionic liquids, Classical Molecular Dynamics, *Ab Initio* Molecular Dynamics, Structural Characterization.

Education

- 1st November, 2008 – 20th April, 2012, L'Aquila, *Italy*
PhD in Environmental and Cultural Heritage Chemistry at the *University of L'Aquila*, with a dissertation on "*Structure of ionic liquids: X-ray scattering and molecular dynamics*".
- 1st October, 2005 – 08th April, 2008, L'Aquila, *Italy*
Master Degree in Chemical Sciences at the *University of L'Aquila* (final mark: 110/110 with honors).
Thesis title: "*Electronic effects and structural variation in monosubstituted benzene rings: the role of intermolecular interactions*".
- 1st October, 2001 – 28th April, 2005, L'Aquila, *Italy*
Bachelor Degree in Chemical Sciences at the *University of L'Aquila* (final mark: 110/110 with honors).
Thesis title: "*Inductive and resonance effect in phenate and anilinium ions: a quantum chemical study of solvent role*".

Research visits and project funding

- 2015– Research Grant from Scuola Normale Superiore, Pisa, Italy.
Title of Project: "The complexity of simplicity: new Force Fields for small but complex molecules".

- 6th April, 2014 – 18th April, 2014
Visiting researcher at Consiglio Nazionale delle Ricerche (CNR), Istituto di Struttura della Materia, Rome, Italy. Research group led by Dr. Alessandro Triolo. Financing COST Action CM1206.
- 1st July, 2010 – 10th December, 2010
Visiting student at TIM (Thermodynamique et Interactions Moléculaires) group, Université Blaise Pascal, Clermont Ferrand, France. Research group led by Prof. Agílio Pádua. Project supported with the scholarship "Reti per l'Alta Formazione", P.O. FSE Abruzzo 2007-2013, D.R. N° 1036/2011 .
- 1st June, 2009 – 30th June, 2010
Visiting student at EDXD (Energy Dispersive X-ray Diffraction) group, Sapienza Università di Roma, Rome, Italy. Research group led by Prof. Ruggero Caminiti.

Schools/Workshops

"Scripting in Python", Consorzio interuniversitario per le Applicazioni di Supercalcolo per Università e Ricerca (CASPUR), Rome (Italy), 25th-28th, October 2011.

"Introduzione al calcolo parallelo con MPI e OpenMP", Consorzio interuniversitario per le Applicazioni di Supercalcolo per Università e Ricerca (CASPUR), Rome (Italy), 17th-19th, May 2011.

"Calcolo Scientifico e tecnico in linguaggio Fortran95", Consorzio interuniversitario per le Applicazioni di Supercalcolo per Università e Ricerca (CASPUR), Rome (Italy), 3rd-6th, May 2011.

"Leuven Summer School of Ionic Liquids", Katholieke Universiteit, Leuven (Belgium), 23rd-27th, August 2010.

"Produttività in ambiente UNIX/Linux", Consorzio interuniversitario per le Applicazioni di Supercalcolo per Università e Ricerca (CASPUR), Rome (Italy), 27th-29th, January 2009.

Conferences

"IV Congresso Nazionale della Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana", Scuola Normale Superiore, Pisa (Italy), 3rd-5th, October 2016.

"Winter Modeling 2015", Scuola Normale Superiore, Pisa (Italy), December 18th, 2015.

"5th Congress on Ionic Liquids", Algarve, Portugal, 21st-25th, April 2013.

Poster: "Investigating the structure of 1-ethyl-3-methylimidazolium tetracyanoborate ionic liquid".

"Quarto Convegno Giovani Chimici", Sapienza Università di Roma, Rome, 16th-17th, June 2010.

Poster: "X-ray scattering and molecular dynamics study of ionic liquids".

"Ionic liquid for Electrochemical Devices-ILED2", Sapienza Università di Roma, Rome, 9th-11th, June 2010.

Poster: "X-ray scattering and molecular dynamics study of liquids 1-ethyl-3-methylimidazolium alkylsulfates".

"Plenty of room at the bottom", Università degli Studi dell'Aquila, L'Aquila, June 7th, 2010.

Oral presentation "Structure of ionic liquids by X-ray scattering and molecular dynamics".

"Winter Modeling 2010", Scuola Normale Superiore, Pisa (Italy), February 26th, 2010.

Poster: "X-ray scattering and molecular dynamics study of liquids 1-alkyl-3-methylimidazolium hexafluorophosphates".

Publications

Macchiagodena M., Mancini G., Pagliai M. Barone V.

"Accurate prediction of bulk properties in hydrogen bonded liquids: amides as case studies."

Phys. Chem. Chem. Phys. **18**, 25342, 2016

Holloczki O., Macchiagodena M., Weber H., Thomas M., Brehm M., Stark A., Russina O., Triolo A., Kirchner B.

"Triphilic Ionic-Liquid Mixtures: Fluorinated and Non-fluorinated Aprotic Ionic-Liquid Mixtures."

ChemPhysChem, **16(15)**, 3325, 2015

Russina O., Macchiagodena M., Kirchner B., Mariani A., Aoun B., Russina M., Caminiti R., Triolo A.

"Association in ethylammonium nitrate-dimethyl sulfoxide mixtures: First structural and dynamical evidences"

J. Non-Cryst. Solids, **407**, 333, 2015

Macchiagodena M., Ramondo F., Gontrani L., Triolo A., Caminiti R.

"Liquid structure of 1-ethyl-3-methylimidazolium alkylsulfates by X-ray scattering and molecular dynamics"

J. Phys. Chem. B, **116**, 13448, 2012

Podgoršek A., Macchiagodena M., Ramondo F., Costa Gomez M. F., Pádua A. H.

"Glycine in 1-butyl-3-methylimidazolium acetate and trifluoroacetate ionic liquids: effect of fluorination and hydrogen bonding"

ChemPhysChem, **13**, 1753, 2012

Macchiagodena M., Gontrani L., Ramondo F., Triolo A., Caminiti R.

"Liquid structure of 1-alkyl-3-methylimidazolium hexafluorophosphates by wide angle X-ray and neutron scattering and molecular dynamics"

J. Chem. Phys., **134**, 114521, 2011

Campanelli A. R., Domenicano A., Macchiagodena M., Ramondo F.

"Electronegativity and resonance parameters from the geometry of monosubstituted benzene rings"

Struct. Chem., **22**, 1131, 2011

Computer skills and competences

UNIX/Linux and Windows, Fortran and awk, Microsoft Office (Word, Excel, PowerPoint, etc.), LaTeX, GAUSSIAN, DLPOLY, VMD, LAMMPS, CP2K, TRAVIS, Orca, Gnuplot, GROMACS.

Language skills

Italian (mother tongue), English (full professional proficiency), French (full professional proficiency), German (limited working proficiency).