Personal Information

First name	Riccardo
Last name	Chelli
Date of birth	28 April 1969
Citizenship	Italian
Title	PhD in Chemistry

Contact Information

Postal Address	Dipartimento di Chimica, Università di Firenze, Via della Lastruccia 3, 50019 Sesto Fiorentino (FI), Italy
E-mail	riccardo.chelli@unifi.it
Telephone	+39-0554573082
Skype	riccardo.chelli1
Home page	www.chim.unifi.it:/u/chelli

Education and Employments

1996	Degree in Chemistry at the University of Firenze (Italy). Thesis title: Structure and rotational dynamics of the NaCN crystal in the plastic phase. Supervisor: Prof. Salvatore Califano. Result: 110/110 cum laude.
2000	PhD in Chemistry at the University of Firenze. Thesis title: Numerical experiments: methods and applications. Supervisor: Prof. Salvatore Califano.
2001 - 2009	Postdoctoral position at the Department of Chemistry of the University of Firenze.
2009 - 2015	Researcher at the Department of Chemistry of the University of Firenze.
2015 - Today	Associate Professor of chemical-physics at the Department of Chemistry of the University of Firenze.

Fellowships, Research Stages and Awards

2000	Special mention in the Semerano Prize by the Chemical-Physics Division of the Italian Chemical Society for the article entitled *Electrical response in chemical potential equalization schemes*, Ref. [95].
2003	Department of Energy Engineering of the University of Firenze. Project title: a physico-mathematical model to study the wax deposition in a boundary layer for a waxy crude oil flowing in a pipe in turbulent regime.
2004	Visiting Researcher at the Dept. of Chemistry of the University of California, Irvine, USA (host Prof. Shaul Mukamel).
2005	International Consortium for Advanced Design of Firenze and Department of Energy Engineering of the University of Firenze. Project title: a FORTRAN parallel code for computational fluid dynamics.
2006	Award for the best poster at the "XXII National Congress of the Italian Chemical Society" (Poster title: *Structure and bonding of water molecules in the polar region of phospholipid membranes investigated by two-dimensional IR spectroscopy and MD simulation*).
2012	Visiting researcher at the Laboratory of Pharmacological and Toxicological Chemistry and Biochemistry of the René Descartes University, Paris, France (host Dr. Nohad Gresh).
2014	Visiting researcher at the Institute of Chemical Physics and Theoretical Chemistry of the Pierre and Marie Curie University, Paris, France (host Prof. Jean-Philip Piquemal).
2014	National Scientific Qualification for the role of Associate Professor in the areas "Modeling and Methods in Chemistry" and "Theoretical Physics of Matter".

Ref. [46]: Article selected by the Editor for the publication on Highlights in Chemical Biology: Research Articles (RSC), number 6, 2008.

Ref. [48]: Article selected by the Editor for the publication on Virtual Journal of Biological Physics Research (AIP & APS), vol. 15, 15 April 2008.

Ref. [58]: Article selected by the Editor for the publication on Virtual Journal of Biological Physics Research (AIP & APS), vol. 12, 1 November 2006.

Ref. [68]: Article selected by the Editor for the publication on Virtual Journal of Biological Physics Research (AIP & APS), vol. 10, 15 July 2005.

Research Interests and Scientific Activity

1. Development of numerical schemes for the phase-space sampling and to compute chemical-physical properties via computer simulations (molecular dynamics and Monte Carlo).
2. Theoretical aspects of nonequilibrium thermodynamics.
3. Development of polarizable force fields for computer simulations.
4. Molecular modeling of systems of biochemical and biophysical interest. Dynamical and structural properties of isolated molecules, molecular clusters and condensed phases via molecular mechanics/dynamics and quantum mechanical calculations.
5. Aspects regarding the correlation between properties at the microscopic level and optical activity of biomolecules and simple liquids, with special attention to the development of models for the interpretation or the prediction of optical spectra.

A bit more detailed description

My scientific background is based on theoretical and computational aspects of the chemistry. Through the years, most of the research interests were addressed to the understanding of the correlation between dynamical and structural properties of condensed systems, with special attention to liquids (Refs. [35, 42, 54, 56, 65, 67, 71, 78, 79, 84, 89, 90, 91, 93, 97, 98, 99, 100]). Such studies were carried out using molecular dynamics (MD) simulations and quantum-mechanical calculations, two computational tools which have been often used during my scientific career. However, my interest was also addressed to more strictly theoretical aspects of the computational chemistry. In this respect, I contributed to develop new methods for the calculation of the elastic neutron scattering and of the constant pressure molar specific heat from the atomic trajectories obtained by MD simulations (Refs. [98, 99]). Since 1999, I was engaged in a research project aimed at the development of empirical potential force fields, with special attention to the development of computational schemes, based on the explicit treatment of the electronic polarization response, for the calculation of electrostatic interactions in classical MD simulations. This research field led to Refs. [52, 64, 68, 70, 72, 80, 81, 86, 95, 96]. Since 2000, I approached theoretico-computational investigations of systems of biochemical interest. Such researches have been mainly addressed to the study of the fundamental interactions occurring between basic biochemical compounds (*i.e.*, model molecules for mimicking the interactions between amino acid side-chains; Refs. [82, 83, 88]) or to the understanding of the mechanisms underlying the protein folding phenomena (Refs. [46, 61, 62, 69, 74, 77]). Several researches have also been carried out on gaseous phases to understand the basic interactions occurring in isolated molecules and clusters of molecules (Refs. [73, 75, 76, 85, 87, 92]). In 2001 I obtained an award (for young researchers) from the University of Firenze to study the thermodynamic properties of prion proteins (Refs. [62, 69]). Since 2005, I realized several studies addressed to methodologies based on nonequilibrium statistical mechanics (Refs. [26, 28, 29, 31, 37, 39, 41, 43, 44, 48, 49, 53, 55, 57, 58]), theoretical aspects of the phase-space sampling in computer simulations (Refs. [25, 34, 38, 40, 59, 66]) and spectroscopic behavior of the matter (Refs. [22, 27, 35, 36, 42, 47, 50, 51, 54, 60, 63]).

I am member of the team for the development of ORAC[40], a program for classical molecular dynamics simulations (http://www.chim.unifi.it/orac).

I am also developer of SIBFA, a program for molecular mechanics calculations using polarizable force fields, developed by the research group of Dr. Nohad Gresh of the Laboratoire de Chimie et Biochimie Pharmacologiques et Toxicologiques of the University Paris Descartes, Paris, France.

Editorial activities

2015 - 2019 Member of the editorial board of the "International Journal of Computational and Theoretical Chemistry" (Science Publishing Group).

2012 - Today Member of the editorial board of the "Journal of Chemistry" (Hindawi Publishing Corporation).

2013 - Today Member of the editorial board of the "Journal of Theoretical and Computational Science" (OMICS Publishing Group).

2019 - Today Member of the editorial board of "Molecules" (MDPI Publishing Group).

Reviewer for the following international scientific journals:

- American Journal of Physical Chemistry
- Biochemistry
- Biophysical Journal
- Carbohydrate Research
- Chemical Physics
- Journal of Chemistry
- International Journal of Molecular Sciences
- Journal of Chemical Physics
- Journal of Chemical Theory and Computation
- Journal of Computational Chemistry
- Journal of Molecular Graphics and Modelling
- Chemical Physics Letters
- Molecular Simulation
- Molecules
- Proteins: Structure, Function, and Bioinformatics
- Journal of Molecular Modeling
- Journal of Physical Chemistry A
- Journal of Physical Chemistry B
- Journal of the American Chemical Society
- Journal of Theoretical and Computational Science
- Letters in Drug Design & Discovery
- Nature Communications
- Physical Chemistry Chemical Physics
- Physics Letters A
- Journal of Computational and Applied Mathematics
- Modelling and Simulation in Materials Science and Engineering
- PLOS ONE
- European Biophysical Journal

Memberships

1997 - Today Member of the European Laboratory for Non-linear Spectroscopy, Sesto Fiorentino, Italy.

2009 - 2014; 2017 - Today Member of the Council of Teachers of the PhD School of Chemistry of the University of Firenze.

2016 - Today Member of the Direction Council of the Department of Chemistry of the University of Firenze.

2016 - Today Member of the Council for Direction Politics and Self-Evaluation of the Department of Chemistry of the University of Firenze.

2019 - Today Member of the Council of the Schoool of Human Health Sciences of the University of Firenze.

Other activities

2002 Engagement in discovering historical sources for a book, entitled *The University of Firenze 1924-2004* (published in 2005), on the history of the University of Firenze.

2009 - 2013 Member of the managing team of the web page of the Department of Chemistry of the University of Firenze.

Teaching Activity

1996 - 1997 Tutor for the course: "Chemistry of the environment". (University of Firenze, Italy).

2002 - 2003 Tutor for the course: "Numerical calculation". (University of Firenze, Italy).

2001 - 2007 Tutor for the course: "Informatics in chemistry". (University of Firenze, Italy).

2009, 2015 - Today Teacher for the course: "Theoretical Chemistry" (Advanced degree in Chemistry, University of Firenze, Italy).

2011 - Today Teacher for the course: "Ceramic and Glass Materials" (First degree in Chemistry, University of Firenze, Italy).

2012 - Today Teacher for the course: "Computational Chemistry" (Advanced degree in Chemical and Pharmaceutical Technologies, University of Firenze, Italy).

2019 - Today Teacher for the course: "Molecular Solids: Structure, Dynamics and Optical and NMR Spectroscopies" (Advanced degree in Chemistry, University of Firenze, Italy).

List of Publications (asterisks indicate Chelli as the corresponding author)

[1] M. Innocenti, A. Giaccherini, R. Chelli, S. Martinuzzi, W. Giurlani, M. Passaponti, A. Lavacchi, C. Fontanesi
Modelling of the elementary steps involved in the Aluminum electrochemical deposition from ionic liquid based solution: the BMImCl/$AlCl_3$ system
Journal of the Electrochemical Society 2020, 167 n. 013525.

[2] V. V. Volkov, R. Chelli, R. Righini, C. C. Perry
Indigo chromophores and pigments: Structure and dynamics

Dyes and Pigments 2020, 172 n. 107761.

[3] F. Nuti, C. Gellini, M. Larregola, L. Squillantini, R. Chelli, P. R. Salvi, O. Lequin, G. Pietraperzia, A. M. Papini
A photochromic azobenzene peptidomimetic of a beta-turn model peptide structure as a conformational switch
Frontiers in Chemistry 2019, 7 n. 180.

[4] M. Pagliai, G. Funghi, D. Vassetti, P. Procacci, R. Chelli, G. Cardini
Imidazole in aqueous solution: hydrogen bond interactions and structural reorganization with concentration
The Journal of Physical Chemistry B 2019, 123 p. 4055–4064.

[5] L. Briccolani-Bandini, A. Brandi, G. Cardini, R. Chelli, F. M. Cordero, C. Gellini, M. Pagliai
Computational investigation of the selective cleavage of diastereotopic cyclopropane bonds in 5-Spirocyclopropane isoxazolidines rearrangement
The Journal of Organic Chemistry 2019, 84 p. 6757–6764.

[6] * E. Giovannelli, C. Gellini, G. Pietraperzia, G. Cardini, P. Procacci, M. Pagliai, V. Volkov, R. Chelli
Correspondence between light-absorption spectrum and nonequilibrium work distribution as a mean to access free energy differences between electronic states
The Journal of Chemical Physics 2018, 149 n. 084101.

[7] G. La Penna, R. Chelli
Structural insights into the osteopontin-aptamer complex by molecular dynamics simulations
Frontiers in Chemistry 2018, 6 n. 2.

[8] * E. Giovannelli, M. Cioni, P. Procacci, G. Cardini, M. Pagliai, V. Volkov, R. Chelli
Binding free energies of host-guest systems by nonequilibrium alchemical simulations with constrained dynamics: Illustrative calculations and numerical validation
Journal of Chemical Theory and Computation 2017, 13 p. 5887–5899.

[9] * E. Giovannelli, P. Procacci, G. Cardini, M. Pagliai, V. Volkov, R. Chelli
Binding free energies of host-guest systems by nonequilibrium alchemical simulations with constrained dynamics: Theoretical framework
Journal of Chemical Theory and Computation 2017, 13 p. 5874–5886.

[10] C. Caratelli, R. Cammi, R. Chelli, M. Pagliai, G. Cardini, V. Schettino
Insights on the realgar crystal under pressure from XP-PCM and periodic model calculations
The Journal of Physical Chemistry A 2017, 121 p. 8825–8834.

[11] L. Moroni, M. Pagliai, R. Chelli, G. Pietraperzia, P. R. Salvi, C. Gellini
Photochemical reactivity of 1,6-methano[20]annulene
The Journal of Physical Chemistry A 2017, 121 p. 4412–4421.

[12] P. Procacci, R. Chelli
Statistical mechanics of ligand-receptor noncovalent association, revisited: Binding site and standard state volumes in modern alchemical theories
Journal of Chemical Theory and Computation 2017, 13 p. 1924–1933.

[13] * E. Giovannelli, G. Cardini, V. Volkov, R. Chelli
Nonequilibrium work theorems applied to transitions between configurational domains
Journal of Statistical Mechanics: Theory and Experiment 2016, 123204 p. 1–23.

[14] V. Volkov, R. Chelli
Resolving capacity of infrared–visible sum frequency generation microscopy to address discrete structural realizations of a protein at interface
Journal of Raman Spectroscopy 2016, 47 p. 828–838.

[15] F. Nerattini, R. Chelli, P. Procacci
II. Dissociation free energies in drug–receptor systems via nonequilibrium alchemical simulations: application to the FK506-related immunophilin ligands
Physical Chemistry Chemical Physics 2016, 18 p. 15005–15018.

[16] * E. Giovannelli, G. Cardini, R. Chelli
Elastic barrier dynamical freezing in free energy calculations: a way to speed up nonequilibrium molecular dynamics simulations by orders of magnitude
Journal of Chemical Theory and Computation 2016, 12 p. 1029–1039.

[17] * E. Giovannelli, G. Cardini, R. Chelli
Simulations in generalized ensembles through noninstantaneous switches
Physical Review E 2015, 92 n. 043310.

[18] * R. Chelli, G. Cardini, E. Giovannelli, G. F. Signorini, P. Procacci
Implementations of nonequilibrium methods for free energy calculations: forthcoming developments of the ORAC molecular dynamics simulation code
VIRT&L-COMM 2015, 7 n. 7.

[19] * E. Giovannelli, G. Cardini, C. Gellini, G. Pietraperzia, R. Chelli
Computing free energy differences of configurational basins
Journal of Chemical Theory and Computation 2015, 11 p. 3561–3571.

[20] V. Volkov, R. Chelli
Polarization entanglement of sum-frequency photons: A tool to probe the markovian limit
Physical Review A 2015, 91 n. 063831.

[21] * E. Giovannelli, G. Cardini, C. Gellini, G. Pietraperzia, R. Chelli
Annealed importance sampling with constant cooling rate
The Journal of Chemical Physics 2015, 142 n. 074102.

[22] R. Chelli, G. Pietraperzia, A. Bencini, C. Giorgi, V. Lippolis, P. R. Salvi, C. Gellini
A fluorescent receptor for halide recognition: clues for the design of anion chemosensors
Physical Chemistry Chemical Physics 2015, 17 p. 10813–10822.

[23] * R. Chelli
About a world where second law of thermodynamics can be violated
Journal of Theoretical and Computational Science 2014, 1 n. e107.

[24] * E. Giovannelli, C. Gellini, G. Pietraperzia, G. Cardini, R. Chelli
Nonequilibrium candidate Monte Carlo simulations with configurational freezing schemes
Journal of Chemical Theory and Computation 2014, 10 p. 4273–4283.

[25] * G. F. Signorini, E. Giovannelli, Y. G. Spill, M. Nilges, R. Chelli
Convective replica-exchange in ergodic regimes
Journal of Chemical Theory and Computation 2014, 10 p. 953–958.

[26] * E. Giovannelli, C. Gellini, G. Pietraperzia, G. Cardini, R. Chelli
Combining path-breaking with bidirectional nonequilibrium simulations to improve efficiency in free energy calculations
The Journal of Chemical Physics 2014, 140 n. 064104.

[27] * S. Puccioni, C. Bazzicalupi, A. Bencini, C. Giorgi, B. Valtancoli, G. De Filippo, V. Lippolis, P. R. Salvi, G. Pietraperzia, R. Chelli, C. Gellini
Tuning the emission properties of fluorescent ligands by changing pH: the unusual case of an acridine-containing polyamine macrocycle
The Journal of Physical Chemistry A 2013, 117 p. 3798–3008.

[28] * P. Nicolini, D. Frezzato, C. Gellini, M. Bizzarri, R. Chelli
Toward quantitative estimates of binding affinities for protein-ligand systems involving large inhibitor compounds: a steered molecular dynamics simulation route
Journal of Computational Chemistry 2013, 34 p. 1561–1576.

[29] * R. Chelli, C. Gellini, G. Pietraperzia, E. Giovannelli, G. Cardini
Path-breaking schemes for nonequilibrium free energy calculations
The Journal of Chemical Physics 2013, 138 n. 214109.

[30] * R. Chelli
Journal of Theoretical and Computational Science: Open Access, A bridge to link knowledge from chemistry, physics, biology and more
Journal of Theoretical and Computational Science 2013, 1 n. e102.

[31] * R. Chelli
Local sampling in steered Monte Carlo simulations decreases dissipation and enhances free energy estimates via nonequilibrium work theorems
Journal of Chemical Theory and Computation 2012, 8 p. 4040–4052.

[32] A. Paarmann, M. Lima, R. Chelli, R. Righini, D. Miller
Excitonic effects in the 2DIR spectra of liquid formamide
in Research in Optical Sciences, OSA Technical Digest (Optical Society of America) 2012, paper IW3D.2.

[33] * R. Chelli, G. F. Signorini
Serial generalized ensemble simulations of biomolecules with self-consistent determination of weights (erratum)
Journal of Chemical Theory and Computation 2012, 8 p. 2552–2552.

[34] * R. Chelli, G. F. Signorini
Serial generalized ensemble simulations of biomolecules with self-consistent determination of weights
Journal of Chemical Theory and Computation 2012, 8 p. 830–842.

[35] A. Paarmann, M. Lima, R. Chelli, V. V. Volkov, R. Righini, R. J. D. Miller
Excitonic effects in two-dimensional vibrational spectra of liquid formamide
Physical Chemistry Chemical Physics 2011, 13 p. 11351–11358.

[36] V. V. Volkov, R. Chelli, F. Muniz-Miranda, R. Righini
Structural properties of a membrane associated anchor dipeptide
The Journal of Physical Chemistry B 2011, 115 p. 5294–5303.

[37] * P. Nicolini, D. Frezzato, R. Chelli
Exploiting configurational freezing in nonequilibrium Monte Carlo simulations
Journal of Chemical Theory and Computation 2011, 7 p. 582–593.

[38] * R. Chelli
Optimal weights in serial generalized-ensemble simulations
Journal of Chemical Theory and Computation 2010, 6 p. 1935–1950.

[39] * P. Nicolini, P. Procacci, R. Chelli
Hummer and Szabo-like potential of mean force estimator for bidirectional nonequilibrium pulling experiments/simulations
The Journal of Physical Chemistry B 2010, 114 p. 9546–9554.

[40] S. Marsili, G. F. Signorini, R. Chelli, M. Marchi, P. Procacci
ORAC: a molecular dynamics simulation program to explore free energy surfaces in biomolecular systems at the atomistic level
Journal of Computational Chemistry 2010, 31 p. 1106–1116.

[41] * P. Nicolini, R. Chelli
Improving fast-switching free energy estimates by dynamical freezing
Physical Review E 2009, 80 n. 041124.

[42] M. Lima, R. Chelli, V. V. Volkov, R. Righini
Two-dimensional infrared spectroscopy of a structured liquid: neat formamide
The Journal of Chemical Physics 2009, 130 n. 204518.

[43] * R. Chelli, P. Procacci
A potential of mean force estimator based on nonequilibrium work exponential averages
Physical Chemistry Chemical Physics 2009, 11 p. 1152–1158.

[44] * R. Chelli
Nonequilibrium work relations for systems subject to mechanical and thermal changes
The Journal of Chemical Physics 2009, 130 n. 054102.

[45] V. Bambagioni, D. Bani, A. Bencini, T. Biver, M. Cantore, R. Chelli, L. Cinci, P. Failli, L. Ghezzi, C. Giorgi, S. Nappini, F. Secco, M. R. Tinè, B. Valtancoli, M. Venturini
Polyamine-polycarboxylate metal complexes with different biological effectiveness as nitric

oxide scavengers. Clues for drug design
Journal of Medicinal Chemistry 2008, 51 p. 3250–3260.

[46] S. Marsili, R. Chelli, V. Schettino, P. Procacci
Thermodynamics of stacking interactions in proteins
Physical Chemistry Chemical Physics 2008, 10 p. 2673–2685.

[47] * R. Chelli, V. V. Volkov, R. Righini
Retrieval of spectral and dynamic properties from two-dimensional infrared pump-probe experiments
Journal of Computational Chemistry 2008, 29 p. 1507–1516.

[48] C. P. Calderon, R. Chelli
Approximating nonequilibrium processes using a collection of surrogate diffusion models
The Journal of Chemical Physics 2008, 128 n. 145103.

[49] * R. Chelli, S. Marsili, P. Procacci
Calculation of the potential of mean force from nonequilibrium measurements via maximum likelihood estimators
Physical Review E 2008, 77 n. 031104.

[50] G. Nannucci, L. Moroni, C. Gellini, R. Chelli, P. R. Salvi, V. Schettino, G. Dellepiane
Fluorescence emissions and torsional conformations in π-conjugated chains of PolyDCHD-HS
The Journal of Physical Chemistry C 2007, 111 p. 17485–17492.

[51] V. V. Volkov, R. Chelli, W. Zhuang, F. Nuti, Y. Takaoka, A. M. Papini, S. Mukamel, R. Righini
Electrostatic interactions in phospholipid membranes revealed by coherent 2D IR spectroscopy
Proceedings of the National Academy of Sciences of the United Staes of America 2007, 104 p. 15323–15327.

[52] J.-P. Piquemal, R. Chelli, P. Procacci, N. Gresh
Key role of the polarization anisotropy of water in modeling classical polarizable force fields
The Journal of Physical Chemistry A 2007, 111 p. 8170–8176.

[53] * R. Chelli, S. Marsili, A. Barducci, P. Procacci
Numerical verification of the generalized Crooks nonequilibrium work theorem for non-Hamiltonian molecular dynamics simulations
The Journal of Chemical Physics 2007, 127 n. 034110.

[54] * D. Račko, R. Chelli, G. Cardini, S. Califano, J. Bartoš
Free volume from molecular dynamics simulations and its relationships to the positron annihilation lifetime spectroscopy
Theoretical Chemistry Accounts 2007, 118 p. 443–448.

[55] * R. Chelli, S. Marsili, A. Barducci, P. Procacci
Generalization of the Jarzynski and Crooks nonequilibrium work theorems in molecular dynamics simulations
Physical Review E 2007, 75 n. 050101(R).

[56] V. Schettino, R. Chelli, S. Marsili, A. Barducci, C. Faralli, M. Pagliai, P. Procacci, G. Cardini
Problems in molecular dynamics of condensed phases
Theoretical Chemistry Accounts 2007, 117 p. 1105–1120.

[57] * R. Chelli, S. Marsili, A. Barducci, P. Procacci
Recovering the Crooks equation for dynamical systems in the isothermal-isobaric ensemble: a strategy based on the equations of motion
The Journal of Chemical Physics 2007, 126 n. 044502.

[58] P. Procacci, S. Marsili, A. Barducci, G. F. Signorini, R. Chelli
Crooks equation for steered molecular dynamics using a Nosé-Hoover thermostat
The Journal of Chemical Physics 2006, 125 n. 164101.

[59] S. Marsili, A. Barducci, R. Chelli, P. Procacci, V. Schettino
Self-healing umbrella sampling: a non equilibrium approach for quantitative free energy calculations
The Journal of Physical Chemistry B 2006, 110 p. 14011–14013.

[60] V. V. Volkov, F. Nuti, Y. Takaoka, R. Chelli, A. M. Papini, R. Righini
Hydration and hydrogen bonding of carbonyls in dimyristoyl-phosphatidylcholine bilayer
Journal of the American Chemical Society 2006, 128 p. 9466–9471.

[61] * R. Chelli, P. Procacci
Comment on "From Subtle to Substantial: Role of Metal Ions on π-π Interactions"
The Journal of Physical Chemistry B 2006, 110 p. 10204–10205.

[62] A. Barducci, R. Chelli, P. Procacci, V. Schettino, F. L. Gervasio, M. Parrinello
Metadynamics simulation of prion protein: β-structure stability and the early stages of misfolding
Journal of the American Chemical Society 2006, 128 p. 2705–2710.

[63] V. V. Volkov, R. Chelli, R. Righini
Domain formation in lipid bilayers probed by two-dimensional infrared spectroscopy
The Journal of Physical Chemistry B 2006, 110 p. 1499–1501.

[64] * R. Chelli, A. Barducci, L. Bellucci, V. Schettino, P. Procacci
Behavior of polarizable models in presence of strong electric fields. I. Origin of nonlinear effects in water-point charge systems
The Journal of Chemical Physics 2005, 123 n. 194109.

[65] M. Paolantoni, R. Chelli, M. Ricci, P. Foggi
Proceedings of the "XI TRVS International Conference": Time Resolved Vibrational Spectroscopy, edito da Salvatore Califano, Paolo Foggi e Roberto Righini.
The ultrafast dynamics of liquid 1-octanol measured by femtosecond optical Kerr effect 2005, p. 211–216.

[66] A. Magro, D. Frezzato, A. Polimeno, G. J. Moro, R. Chelli, R. Righini
Dynamics of liquid benzene: a cage analysis
The Journal of Chemical Physics 2005, 123 n. 124511.

[67] * R. Chelli, R. Righini, S. Califano
Structure of liquid formic acid investigated by first principle and classical molecular dynamics simulations
The Journal of Physical Chemistry B 2005, 109 p. 17006–17013.

[68] * R. Chelli, V. Schettino, P. Procacci
Comparing polarizable force fields to ab initio calculations reveals nonclassical effects in condensed phases
The Journal of Chemical Physics 2005, 122 n. 234107.

[69] * A. Barducci, R. Chelli, P. Procacci, V. Schettino
Misfolding pathways of the prion protein probed by molecular dynamics simulations
Biophysical Journal 2005, 88 p. 1334–1343.

[70] * R. Chelli, M. Pagliai, P. Procacci, G. Cardini, V. Schettino
Polarization response of water and methanol investigated by a polarizable force field and density functional theory calculations: implications for charge transfer
The Journal of Chemical Physics 2005, 122 n. 074504.

[71] * D. Račko, R. Chelli, G. Cardini, J. Bartoš, S. Califano
Insights into positron annihilation lifetime spectroscopy by molecular dynamics simulations. Free-volume calculations for liquid and glassy glycerol
European Physical Journal D 2005, 32 p. 289–297.

[72] * R. Chelli, P. Procacci
Comment to "Calculation of the Dipole Moment for Polypeptides Using the Generalized Born-Electronegativity Equalization Method: Results in Vacuum and Continuum-Dielectric Solvent"
The Journal of Physical Chemistry B 2004, 108 p. 16995–16997.

[73] G. Pietraperzia, R. Chelli, M. Becucci, A. Riganelli, M. Alberti, A. Laganà
Molecular mechanics and dynamics calculations to bridge molecular structure information and spectroscopic measurements on complexes of aromatic compounds
Lecture Notes in Computer Science 2004, 3044 p. 374–382.

[74] * G. F. Signorini, R. Chelli, P. Procacci, V. Schettino
Energetic fitness of histidine protonation states in PDB structures
The Journal of Physical Chemistry B 2004, 108 p. 12252–12257.

[75] M. Becucci, G. Pietraperzia, M. Pasquini, G. Piani, A. Zoppi, R. Chelli, E. Castellucci, W. Demtroeder
A study on the anisole-water complex by molecular beam-electronic spectroscopy and molecular mechanics calculations
The Journal of Chemical Physics 2004, 120 p. 5601–5607.

[76] A. S. Gemechu, L. J. H. Hoffmann, S. Marquardt, C. G. Eisenhardt, H. Baumgärtel, R. Chelli, G. Cardini, S. Califano
The absorption spectrum of anisole and the anisole/CO_2 1:1-cluster. The influence of intermolecular interaction on intramolecular vibrations
Zeitschrift für Physikalische Chemie: International journal of research in physical chemistry and chemical physics 2004, 218 p. 123–153.

[77] * R. Chelli, F. L. Gervasio, P. Procacci, V. Schettino
Inter-residue and solvent-residue interactions in proteins: a statistical study on experimental structures
Proteins: Structure, Function, and Bioinformatics 2004, 55 p. 139–151.

[78] * R. Chelli, G. Cardini, P. Procacci, R. Righini, S. Califano
Proceedings of the "XII UPS Conference": Recent Advances in Ultrafast Spectroscopy, edito da Salvatore Califano, Paolo Foggi e Roberto Righini.
Dynamics and structure of liquid and supercooled liquid m-toluidine investigated by molecular dynamics simulations 2003, p. 57–67.

[79] R. Chelli, G. Cardini, P. Procacci, R. Righini, S. Califano
Dynamical and structural correlation in supercooled liquids: a molecular dynamics investigation of m-toluidine
The Journal of Chemical Physics 2003, 119 p. 357–363.

[80] * R. Chelli, P. Procacci
Comment on "Classical polarizable force fields parametrized from ab initio calculations" [J. Chem. Phys. 117, 1416 (2002)]
The Journal of Chemical Physics 2003, 118 p. 1571–1572.

[81] R. Chelli, P. Procacci
A transferable polarizable electrostatic force field for molecular mechanics based on the chemical potential equalization principle
The Journal of Chemical Physics 2002, 117 p. 9175–9189.

[82] F. L. Gervasio, R. Chelli, P. Procacci, V. Schettino
The nature of intermolecular interactions between aromatic amino acid residues
Proteins: Structure, Function, and Genetics 2002, 48 p. 117–125.

[83] R. Chelli, F. L. Gervasio, P. Procacci, V. Schettino
Stacking and T-shape competition in aromatic-aromatic amino acid interactions
Journal of the American Chemical Society 2002, 124 p. 6133–6143.

[84] R. Chelli, G. Cardini, P. Procacci, R. Righini, S. Califano
Molecular dynamics of glass-forming liquids: structure and dynamics of liquid metatoluidine
The Journal of Chemical Physics 2002, 116 p. 6205–6215.

[85] F. L. Gervasio, R. Chelli, P. Procacci, V. Schettino
Is the T-shaped toluene dimer a stable intermolecular complex?
The Journal of Physical Chemistry A 2002, 106 p. 2945–2948.

[86] R. Chelli, R. Righini, S. Califano, P. Procacci
Towards a polarizable force field for molecular liquids
Journal of Molecular Liquids 2002, 96-97 p. 87–100.

[87] C. G. Eisenhardt, A. S. Gemechu, H. Baumgärtel, R. Chelli, G. Cardini, S. Califano
Excited state photoelectron spectroscopy of anisole
Physical Chemistry Chemical Physics 2001, 3 p. 5358–5368.

[88] F. L. Gervasio, R. Chelli, M. Marchi, P. Procacci, V. Schettino
Determination of the potential of mean force of aromatic amino acid complexes in various solvents using molecular dynamics simulations: The case of the tryptophan-histidine pair
The Journal of Physical Chemistry B 2001, 105 p. 7835–7846.

[89] R. Chelli, G. Cardini, M. Ricci, P. Bartolini, R. Righini, S. Califano
The fast dynamics of benzene in the liquid phase. Part II: A molecular dynamics simulation
Physical Chemistry Chemical Physics 2001, 3 p. 2803–2810.

[90] M. Ricci, P. Bartolini, R. Chelli, G. Cardini, S. Califano, R. Righini
The fast dynamics of benzene in the liquid phase. Part I: Optical Kerr effect experimental investigation
Physical Chemistry Chemical Physics 2001, 3 p. 2795–2802.

[91] R. Chelli, G. Cardini, P. Procacci, R. Righini, S. Califano, A. Albrecht
Simulated structure, dynamics, and vibrational spectra of liquid benzene
The Journal of Chemical Physics 2000, 113 p. 6851–6863.

[92] R. Chelli, F. L. Gervasio, C. Gellini, P. Procacci, G. Cardini, V. Schettino
Conformational distribution of gas-phase glycerol
The Journal of Physical Chemistry A 2000, 104 p. 11220–11222.

[93] R. Chelli, F. L. Gervasio, C. Gellini, P. Procacci, G. Cardini, V. Schettino
Density functional calculation of structural and vibrational properties of glycerol
The Journal of Physical Chemistry A 2000, 104 p. 5351–5357.

[94] * R. Chelli, S. Ciabatti, G. Cardini, R. Righini, P. Procacci
Erratum: "Calculation of optical spectra in liquid methanol using molecular dynamics and the chemical potential equalization method" [J. Chem. Phys. 111, 4218, (1999)]
The Journal of Chemical Physics 2000, 112 p. 5515–5515.

[95] * R. Chelli, P. Procacci, R. Righini, S. Califano
Electrical response in chemical potential equalization schemes
The Journal of Chemical Physics 1999, 111 p. 8569–8575.

[96] * R. Chelli, S. Ciabatti, G. Cardini, R. Righini, P. Procacci
Calculation of optical spectra in liquid methanol using molecular dynamics and the chemical potential equalization method
The Journal of Chemical Physics 1999, 111 p. 4218–4229.

[97] R. Chelli, P. Procacci, G. Cardini, S. Califano
Glycerol condensed phases. Part II. A molecular dynamics study of the conformational structure and hydrogen bonding
Physical Chemistry Chemical Physics 1999, 1 p. 879–885.

[98] * R. Chelli, P. Procacci, G. Cardini, R. G. Della Valle, S. Califano
Glycerol condensed phases. Part I. A molecular dynamics study
Physical Chemistry Chemical Physics 1999, 1 p. 871–877.

[99] R. Chelli, G. Cardini, S. Califano
Calculation of elastic coherent neutron scattering spectra from molecular dynamics data: the NaCN plastic crystal
Chemical Physics Letters 1997, 274 p. 335–340.

[100] R. Chelli, G. Cardini, S. Califano
A molecular dynamics study of translation-rotation coupling in the NaCN plastic crystal
The Journal of Chemical Physics 1997, 107 p. 8041–8050.