Marcello Sega — Curriculum vitae

Personal Data

Name Marcello Sega
Birth date October 25, 1977
Birth place Bolzano, Italy

Contact

Languages Italian (native), English (full professional proficiency), German (professional proficiency)

Area of Research

Theoretical and computational soft matter.
The focus of my research is on complex fluids, with particular emphasis on fluid interfaces, and systems of biological interest, from the single molecule level to that of supramolecular aggregates. I develop and make intensive use of advanced simulation approaches, both at the atomistic and at the coarse-grained level.

Current Position

2018–today : Group Leader, Helmholtz Institute Erlangen-Nürnberg

Professional Experience

2015 – 2018 : University Assistant, Computational Physics Group, University of Vienna
2015 – 2018 : Associate Editor, RSC Advances, Royal Society of Chemistry
2013 – 2015 : Marie Curie Fellow, Dept. of Computational Biological Chemistry, University of Vienna
2012 – 2013 : Research Assistant, Physics Dept., University of Rome "Tor Vergata"
2010 – 2012 : Postodc, ICP, University of Stuttgart
2008– 2010 : Research Assistant, Physics Dept., University of Trento
2006–2008 : Postdoc, FIAS, J.W. Goethe University, Frankfurt am Main
2005–2006 : Research Assistant, Physics Dept., University of Trento

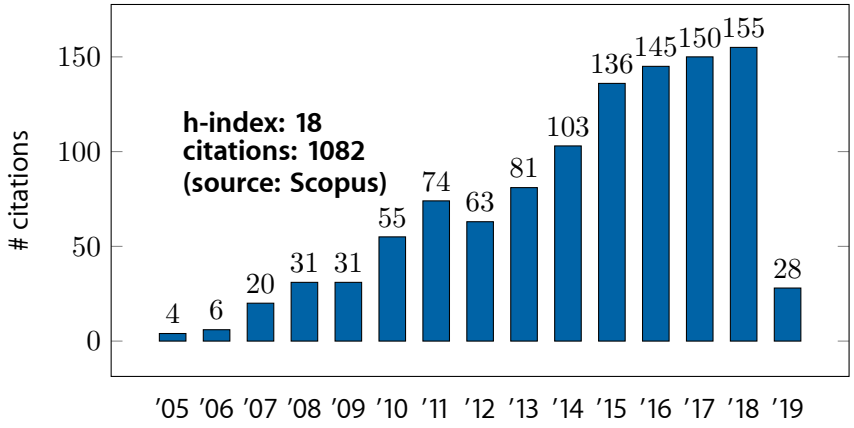
Education

2017 : Habilitation – Computational Physics, University of Vienna (Austria),
"Simulation of Interfaces and Flows from the Nano to the Mesoscale"
2005 : Ph.D. – Physics, University of Trento (Italy),
"Structural and Dynamical Properties of a GM3 Bilayer Studied by Computer Simulation"
2001 : Laurea (Master equivalent) – Physics, University of Trento (Italy), 110/110 with distinction
"Study of the dynamical properties of polymers in solution by means of numerical simulation techniques."

Major Funded Projects

2015 – 2018 : EU-H2020 ITN-ETN grant 642774 "COLLDENSE", PI of the project "Complex solutes at liquid-liquid interfaces", University of Vienna node.
Project Budget: 255.000 €, whole network: 3.895.000 €
2013 – 2015 : EU-FP7 Marie Curie IEF grant 331932 "SIDIS", "Simulation of Dielectric Spectra"
Budget: 248.000 €

Publication Metrics



Activity: 2004 – today, 63 peer reviewed publications
Scopus: `https://www.scopus.com/authid/detail.uri?authorId=6701682678`
Thomson Reuters: `http://www.researcherid.com/rid/C-8863-2009`
ORCID: `http://orcid.org/0000-0002-0031-905X`

Invited talks at conferences and seminars

11.2017 Bio-Soft-Matter Special Seminar, Freie Universität Berlin, *Intrinsic properties of fluid-fluid interfaces*
03.2016 NIH, National Heart, Lung, and Blood Institute, Bethesda, *The intrinsic structure of liquid interfaces*
03.2014 SMU Dallas, 25th Austin Symposium, *The dielectric spectrum of water and Hubbard-Onsager kinetic decrement*
12.2011 ETH-Z, Competence Center for Computational Chemistry (C4), *Computing Dielectric Properties of Charged Soft-Matter*
09.2011 NATO Advanced Research Workshop, Perpignan: "Broadband Dielectric Spectroscopy and its Advanced Technological Applications"
05.2008 Nanostructured Bio-interfaces Workshop, Portoroz. *Simulating soft condensed-matter systems at the micron scale*.
04.2008 SISSA, Trieste. *Bridging gaps in soft condensed matter simulations*.
11.2006 SISSA, Trieste. *Searching for dominant folding pathways by computer simulation*.
12.2005 Institute Pasteur, Paris. *Molecular dynamics simulation of ganglioside aggregates*.
05.2004 Eötvös Loránd University, Budapest. *Computer simulation of a Ganglioside bilayer*.

Activities

Organization of Conferences and Workshops

- CECAM Workshop (organiser) "Physics and Chemistry at Fluid/Fluid Interfaces", Vienna, December 2017, 30 participants
- EMLG 2017 (organiser) Conference of the European Molecular Liquids Group (Vienna, September 2017) $\sim$ 100 participants
- MECO 41 (organiser) Conference of the Middle European Cooperation in Statistical Physics (Vienna, February 2016) $\sim$ 150 participants
- ÖPG 2016 (member of the organising commitee) Meeting of the Austrian Physical Society (Vienna, September 2016) $\sim$ 300 participants
- ICMF14 (member of the organising committee) International Conference on Magnetic Fluids (Sverdlovsk, July 2016) $\sim$ 250 participants

Functions in Scientific Associations

- Board Member: European Molecular Liquids Group (treasurer, 2014-today)
- Austrian MC Substitute: COST Action MP1305 "Flowing Matter" (2014-today)
- Austrian MC Substitute: COST Action CM1206 "Exchange on Ionic Liquids" (2015-today)

Editorial Activity

- Associate Editor, RSC Advances (IF: 3.8), Royal Society of Chemistry (2015-today)

Referee

Phys. Rev. Lett. ; JACS ; Soft Matter; Phys. Chem. Chem. Phys.; J. Phys. Chem.; J. Chem. Phys; Phys. Rev. E ; Phys. Rev. Applied; Phys. Fluids; J. Polymer Sci.; J. Mol. Liq.; J. Chem. Theory Computat.;
Full activity on: `http://publons.com/author/256509/`

International collaborations

M. Sbragaglia, L. Biferale, Tor Vergata University, Rome, Italy
C. Holm, University of Stuttgart, Germany
P. Jedlovszky, Eszterhazy Karoly University, Eger, Hungary
S. Melchionna, S. Succi, IAC-CNR, Rome, Italy
F. Pederiva, P. Faccioli, G. Guella, University of Trento, Italy
P. Brocca, L. Cantù, LITA, Milan, Italy
M. Jorge, University of Strathclyde, Glasgow, U.K.

Teaching

Courses

University of Vienna

2017 Computational Physics I Problem Class, exercises, 4 hrs/week, winter semester

2017 Introduction to Physics IV – solid state physics, exercises, 1 hr/week, summer semester

2017 Computational Physics II Problem Class, exercises, 2 hrs/week, summer semester

2017 Tutor for Internship "Scientific Computing"

2016 Computational Physics I Problem Class, exercises, 4 hrs/week, winter semester

2016 Introduction to calculation methods in physics, exercises, 2 hrs/week, winter semester

2016 Introduction to Physics IV – solid state physics, exercises, 2 hr/week, summer semester

2016 Computational Physics II Problem Class, exercises, 2 hrs/week, summer semester

2016 Tutor for Internship "Scientific Computing", summer semester

2015 Computational Physics I Problem Class, exercises, 4 hrs/week, winter semester

2015 Theoretical Physics for the Teacher accred. progr., exercises, 2 hrs/week, winter semester

2015 Hydrodynamics, lecture, 2 hrs/week, summer semester

2014 Theoretical Physics for the Teacher accred. progr., exercises, 2 hrs/week, winter semester

University of Stuttgart

2011 Simulation Methods, exercises, 2 hrs/week, winter semester

2011 Simulation Methods, exercises, 2 hrs/week, summer semester

2010 Simulation Methods, exercises, 2 hrs/week, winter semester

University of Trento

2010 "Fisica II" (electromagnetism lab course, Biotecnologies) 15/02/2010 – 28/05/2010

2003 "Fisica generale 4a unità" (electromagnetism and relativity) 22/09/2003 – 22/11/2003

2002 "Fisica generale 5a unità" (electromagnetism and relativity) 23/09/2002 – 04/04/2003

2002 "Fisica generale II" (electromagnetism) 25/02/2002 – 08/06/2002

Lectures at Workshops/Summer Schools:

2013 *CECAM Workshop ESPResSoSummer School*: lecture and hands-on on two-phase flows

2011 *Computer Modeling of Complex Liquids in ESPREsSo*, Ural State University, Ekaterinburg, Russia.

2009 *Computer Modeling of Complex Liquids in ESPREsSo*, Ural State University, Ekaterinburg, Russia.

2006 *Molecular Dynamics simulations of biological systems*, European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Trento, Italy.

Master and Ph.D. Theses, supervision / co-supervision

Andrei Bazarenko PhD student: 2015-today, University of Vienna (supervisor)

Elija Feigl Master student: 2017-today, University of Vienna (supervisor)

Shervin Rafatnia PhD Physics: 2010-2013, ICP, Stuttgart (co-supervisor)

Emmanuel Autieri PhD Physics: 2009-2011, **University of Trento**, *"Development of free energy calculation methods for the study of monosaccharides conformation in computer simulations"* (co-supervisor)

Kate Clements MSci Physics: 2009, **London Imperial College** and **University of Trento**, *"The Free Energy of Molecular Membrane Transport"* (co-supervisor)

Mehmet Süzen PhD Physics: 2008-2010, FIAS, Frankfurt (co-supervisor)

Alice Lonardi Master Physics: 2008, **University of Trento**, *"Dominant Folding Pathway of a Beta Hairpin"* (co-supervisor)

List of peer reviewed publications in international journals

[1] G. Hantal, B. Fábián, M. Sega, B. Jójárt, and P. Jedlovszky, "Effect of general anesthetics on the properties of lipid membranes of various compositions", Biochim. Biophys. Acta **1861**, 594–609 (2019).

[2] A. Bazarenko and M. Sega, "A simple approximation for the distribution of ions between charged plates in the weak coupling regime", J. Mol. Liq. **271**, 301–304 (2018).

[3] A. Bazarenko and M. Sega, "Electrokinetic droplet transport from electroosmosis to electrophoresis", Soft matter **14**, 9571–9576 (2018).

[4] M. Sega, B. Fabian, G. Hantal, and P. Jedlovszky, "Pytim: a python package for the interfacial analysis of molecular simulations", J. Comput. Chem. **39**, 2118–2125 (2018).

[5] M. Sega, G. Horvai, and P. Jedlovszky, "On the calculation of the surface entropy in computer simulation", J. Mol. Liq. **262**, 58–62 (2018).

[6] M. Sega and P. Jedlovszky, "The impact of tensorial temperature on equilibrium thermodynamics", Phys. Chem. Chem. Phys. **10**, 16910–16912 (2018).

[7] B. Fabian, M. Sega, G. Horvai, and P. Jedlovszky, "Single Particle Dynamics at the Intrinsic Surface of Various Apolar, Aprotic Dipolar, and Hydrogen Bonding Liquids As Seen from Computer Simulations", J. Phys. Chem. B **121**, 5582–5594 (2017).

[8] B. Fábián, M. Sega, V. P. Voloshin, N. N. Medvedev, and P. P. Jedlovszky, "Lateral Pressure Profile and Free Volume Properties in Phospholipid Membranes Containing Anesthetics", J. Phys. Chem. B **121**, 2814–2824 (2017).

[9] M. Sega and C. Dellago, "Long-Range Dispersion Effects on the Water/Vapor Interface Simulated Using the Most Common Models", J. Phys. Chem. B **121**, 3798–3803 (2017).

[10] M. Sega, B. Fabian, A. R. Imre, and P. Jedlovszky, "Relation between the Liquid Spinodal Pressure and the Lateral Pressure Profile at the Liquid-Vapor Interface", J. Phys. Chem. C **121**, 12214–12219 (2017).

[11] M. Sega, B. Fábián, and P. Jedlovszky, "Nonzero Ideal Gas Contribution to the Surface Tension of Water", J. Phys. Chem. Lett. **8**, 2608–2612 (2017).

[12] M. Sega and G. Hantal, "Phase and interface determination in computer simulations of liquid mixtures with high partial miscibility", Phys. Chem. Chem. Phys. **19**, 18968–18974 (2017).

[13] A. Montessori, C. A. Amadei, G. Falcucci, M. Sega, C. D. Vecitis, and S. Succi, "Extended friction elucidates the breakdown of fast water transport in graphene oxide membranes", Europhys. Lett. **116**, 54002–7 (2016).

[14] P. A. Sánchez, J. Smiatek, B. Qiao, M. Sega, and C. Holm, "High Performance Computing in Science and Engineering ´15", in , edited by E. W. Nagel, H. D. Kröner, and M. M. Resch (Springer International Publishing, Cham, 2016) Chap. Atomistic Simulation of Oligoelectrolyte Multilayers Growth, pp. 215–228.

[15] M. Sega, "The role of a small-scale cutoff in determining molecular layers at fluid interfaces", Phys. Chem. Chem. Phys. **68**, 3713–3716 (2016).

[16] M. Sega, B. Fábián, G. Horvai, and P. Jedlovszky, "How Is the Surface Tension of Various Liquids Distributed along the Interface Normal?", J. Phys. Chem. C **120**, 27468–27477 (2016).

[17] M. Sega, B. Fábián, and P. Jedlovszky, "Pressure Profile Calculation with Mesh Ewald Methods", J. Chem. Theory Comput., 4509–4515 (2016).

[18] B. Fabian, M. Darvas, S. Picaud, M. Sega, and P. Jedlovszky, "The effect of anaesthetics on the properties of a lipid membrane in the biologically relevant phase: a computer simulation study", Phys. Chem. Chem. Phys. **17**, 14750–14760 (2015).

[19] G. Hantal, M. Sega, S. Kantorovich, C. Schroeder, and M. Jorge, "Intrinsic Structure of the Interface of Partially Miscible Fluids: An Application to Ionic Liquids", J. Phys. Chem. C **119**, 28448–28461 (2015).

[20] M. Sega, B. Fabian, and P. Jedlovszky, "Layer-by-layer and intrinsic analysis of molecular and thermodynamic properties across soft interfaces", J. Chem. Phys. **143**, 114709 (2015).

[21] M. Sega, M. Sbragaglia, L. Biferale, and S. Succi, "The importance of chemical potential in the determination of water slip in nanochannels", Eur. Phys. J. E **38**, 1–7 (2015).

[22] M. Sega and C. Schröder, "Dielectric and Terahertz Spectroscopy of Polarizable and Nonpolarizable Water Models: A Comparative Study", J. Phys. Chem. A **119**, 1539–1547 (2015).

[23] M. Sega, S. Kantorovich, and A. Arnold, "Kinetic dielectric decrement revisited: phenomenology of finite ion concentrations", Phys. Chem. Chem. Phys. **17**, 130–133 (2015).

[24] P. T. Kiss, M. Sega, and A. Baranyai, "Efficient Handling of Gaussian Charge Distributions: An Application to Polarizable Molecular Models", J. Chem. Theory Comput. **10**, 5513–5519 (2014).

[25] S. Micciulla, P. A. Sanchez, J. Smiatek, B. Qiao, M. Sega, A. Laschewsky, C. Holm, and R. von Klitzing, "Layer-by-Layer Formation of Oligoelectrolyte Multilayers: A Combined Experimental and Computational Study", Soft Mater. **12**, S14–S21 (2014).

[26] S. Raafatnia, O. A. Hickey, M. Sega, and C. Holm, "Computing the Electrophoretic Mobility of Large Spherical Colloids by Combining Explicit Ion Simulations with the Standard Electrokinetic Model", Langmuir **30**, 1758–1767 (2014).

[27] C. Schroeder, M. Sega, M. Schmollngruber, E. Gailberger, D. Braun, and O. Steinhauser, "On the collective network of ionic liquid/water mixtures. IV. Kinetic and rotational depolarization", J. Chem. Phys. **140**, 204505 (2014).

[28] M. Sega, S. S. Kantorovich, C. Holm, and A. Arnold, "Communication: Kinetic and pairing contributions in the dielectric spectra of electrolyte solutions", J. Chem. Phys. **140** (2014) 10.1063/1.4880237.

[29] M. Sega, G. Horvai, and P. Jedlovszky, "Microscopic origin of the surface tension anomaly of water", Langmuir **30**, 2969–2972 (2014).

[30] M. Sega, G. Horvai, and P. Jedlovszky, "Two-dimensional percolation at the free water surface and its relation with the surface tension anomaly of water", J. Chem. Phys. **141**, 54707 (2014).

[31] M. Darvas, M. Jorge, M. N. D. S. Cordeiro, S. S. Kantorovich, M. Sega, and P. Jedlovszky, "Calculation of the Intrinsic Solvation Free Energy Profile of an Ionic Penetrant Across a Liquid-Liquid Interface with Computer Simulations", J. Phys. Chem. B **117**, 16148–16156 (2013).

[32] M. Sega, S. S. Kantorovich, A. Arnold, and C. Holm, "On the calculation of the dielectric properties of liquid ionic systems", in *Nato sci. peace secur. ser. b phys. biophys.* (Springer Netherlands, 2013), pp. 103–122.

[33] M. Sega, S. S. Kantorovich, P. Jedlovszky, and M. Jorge, "The generalized identification of truly interfacial molecules (ITIM) algorithm for nonplanar interfaces", J. Chem. Phys. **138**, 044110 (2013).

[34] M. Sega, M. Sbragaglia, L. Biferale, and S. Succi, "Regularization of the slip-length divergence in water nanoflows by inhomogeneities at the Angstrom scale", Soft Matter, 8526–8531 (2013).

[35] M. Sega, M. Sbragaglia, S. S. Kantorovich, and A. O. Ivanov, "Mesoscale structures at complex fluid-fluid interfaces: a novel lattice Boltzmann/molecular dynamics coupling", Soft Matter **9**, 10092–10107 (2013).

[36] I. Semenov, S. Raafatnia, M. Sega, V. Lobaskin, C. Holm, and F. Kremer, "Electrophoretic mobility and charge inversion of a colloidal particle studied by single-colloid electrophoresis and molecular dynamics simulations", Phys. Rev. E **87**, 022302–7 (2013).

[37] M. Darvas, P. N. M. Hoang, S. Picaud, M. Sega, and P. Jedlovszky, "Anesthetic molecules embedded in a lipid membrane: a computer simulation study", Phys. Chem. Chem. Phys. **14**, 12956–12969 (2012).

[38] S. Kesselheim, M. Sega, and C. Holm, "Effects of dielectric mismatch and chain flexibility on the translocation barriers of charged macromolecules through solid state nanopores", Soft Matter **8**, 9480 (2012).

[39] B.-F. Qiao, M. Sega, and C. Holm, "Properties of water in the interfacial region of a polyelectrolyte bilayer adsorbed onto a substrate studied by computer simulations", Phys. Chem. Chem. Phys. **14**, 11425–11432 (2012).

[40] E. Autieri, E. Chiessi, A. Lonardi, G. Paradossi, and M. Sega, "Conformation and Dynamics of Poly(N-isopropyl acrylamide) Trimers in Water: A Molecular Dynamics and Metadynamics Simulation Study", J. Phys. Chem. B **115**, 5827–5839 (2011).

[41] S. A. Beccara, P. Faccioli, M. Sega, F. Pederiva, G. Garberoglio, and H. Orland, "Dominant folding pathways of a peptide chain from ab initio quantum-mechanical simulations", J. Chem. Phys. **134**, 024501 (2011).

[42] S. Kesselheim, M. Sega, and C. Holm, "Applying ICC* to DNA translocation. Effect of dielectric boundaries", Comput. Phys. Commun. **182**, 33–35 (2011).

[43] B. Qiao, M. Sega, and C. Holm, "An atomistic study of a poly(styrene sulfonate)/poly(diallyldimethylammonium) bilayer: the role of surface properties and charge reversal", Phys Chem Chem Phys **13**, 16336–16342 (2011).

[44] M. Sega, E. Autieri, and F. Pederiva, "Pickett angles and Cremer–Pople coordinates as collective variables for the enhanced sampling of six-membered ring conformations", Mol. Phys. **109**, 141–148 (2011).

[45] E. Autieri, M. Sega, F. Pederiva, and G. Guella, "Puckering free energy of pyranoses: A NMR and metadynamics-umbrella sampling investigation", J. Chem. Phys. **133**, 095104 (2010).

[46] S. Tyagi, M. Süzen, M. Sega, M. Barbosa, S. S. Kantorovich, and C. Holm, "An iterative, fast, linear-scaling method for computing induced charges on arbitrary dielectric boundaries", J. Chem. Phys. **132**, 154112 (2010).

[47] E. Autieri, P. Faccioli, M. Sega, F. Pederiva, and H. Orland, "Dominant reaction pathways in high-dimensional systems", J. Chem. Phys. **130**, 064106 (2009).

[48] M. Sega, E. Autieri, and F. Pederiva, "On the calculation of puckering free energy surfaces", J. Chem. Phys. **130**, 225102 (2009).

[49] M. Sega, R. Vallauri, P. Jedlovszky, M. Sega, and R. Vallauri, "GM1 Ganglioside Embedded in a Hydrated DOPC Membrane : A Molecular Dynamics", J. Phys. Chem. B **113**, 4876–4886 (2009).

[50] J. Smiatek, M. Sega, C. Holm, U. D. Schiller, and F. Schmid, "Mesoscopic simulations of the counterion-induced electro-osmotic flow: A comparative study", J. Chem. Phys. **130**, 244702 (2009).

[51] M. Süzen, M. Sega, and C. Holm, "Ensemble inequivalence in single-molecule experiments", Phys. Rev. E **79**, 1–9 (2009).

[52] P. Faccioli, M. Sega, F. Pederiva, and H. Orland, "Stochastic dynamics and dominant protein folding pathways", Philos. Mag. **88**, 4093–4099 (2008).

[53] L. B. Pártay, M. Sega, and P. Jedlovszky, "A Two-step Aggregation Scheme of Bile Acid Salts, as Seen From Computer Simulations", Prog. Colloid Polym. Sci. **135**, edited by Z. Hórvölgyi and É. Kiss, 181–187 (2008).

[54] L. B. Partay, M. Sega, and P. Jedlovszky, "Counterion binding in the aqueous solutions of bile acid salts, as studied by computer simulation methods", Langmuir **24**, 10729–10736 (2008).

[55] G. Garberoglio, M. Sega, and R. Vallauri, "Inhomogeneity effects on the structure and dynamics of water at the surface of a membrane: A computer simulation study", J. Chem. Phys. **126**, 125103 (2007).

[56] L. B. Pártay, P. Jedlovszky, M. Sega, L. B. Partay, P. Jedlovszky, and M. Sega, "Molecular aggregates in aqueous solutions of bile acid salts. Molecular dynamics simulation study", J. Phys. Chem. B **111**, 9886–9896 (2007).

[57] L. B. Partay, M. Sega, P. P. Jedlovszky, L. B. Pártay, M. Sega, and P. P. Jedlovszky, "Morphology of bile salt micelles as studied by computer simulation methods", Langmuir **23**, 12322–12328 (2007).

[58] M. Sega, P. Faccioli, F. Pederiva, G. Garberoglio, and H. Orland, "Quantitative protein dynamics from dominant folding pathways", Phys. Rev. Lett. **99**, 1–4 (2007).

[59] M. Sega, G. Garberoglio, P. Brocca, and L. Cantu, "Microscopic structure of phospholipid bilayers: Comparison between molecular dynamics simulations and wide-angle X-ray spectra", J. Phys. Chem. B **111**, 2484–2489 (2007).

[60] M. Sega, R. Vallauri, P. Brocca, L. Cantù, and S. Melchionna, "Short-range structure of a GM3 ganglioside membrane: Comparison between experimental WAXS and computer simulation results", J. Phys. Chem. B **111**, 10965–10969 (2007).

[61] P. Faccioli, M. Sega, F. Pederiva, and H. Orland, "Dominant pathways in protein folding", Phys. Rev. Lett. **97**, 108101 (2006).

[62] M. Sega, P. Jedlovszky, and R. Vallauri, "Molecular dynamics simulation of GM1 gangliosides embedded in a phospholipid membrane", J. Mol. Liq. **129**, 86–91 (2006).

[63] M. Sega, R. Vallauri, P. Brocca, and S. Melchionna, "Molecular dynamics simulation of a GM3 ganglioside bilayer (vol 108B, pg 20322, 2004)", J. Phys. Chem. B **109**, 6036 (2005).

[64] M. Sega, R. Vallauri, and S. Melchionna, "Diffusion of water in confined geometry: The case of a multilamellar bilayer", Phys. Rev. E **72**, 3–6 (2005).

[65] M. Sega, P. Jedlovszky, N. N. Medvedev, and R. Vallauri, "Free volume properties of a linear soft polymer: A computer simulation study", J. Chem. Phys. **121**, 2422–2427 (2004).

[66] M. Sega, R. Vallauri, P. Brocca, and S. Melchionna, "Molecular dynamics simulation of a GM3 ganglioside bilayer", J. Phys. Chem. B **108**, 20322–20330 (2004).