

# Marcello Segà — Curriculum vitae

## Personal Data

<b>Name</b>	Marcello Segà	<b>Contact</b>	m.sega@fz-juelich.de
<b>Birth date</b>	October 25, 1977		Helmholtz-Institut Erlangen-Nürnberg
<b>Birth place</b>	Bolzano, Italy		Fürther Straße 248, 90429 Nürnberg, Germany
<b>Languages</b>	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  
2015–today : Associate Editor, RSC Advances, Royal Society of Chemistry

## Professional Experience

2015–2018 : University Assistant, Computational Physics Group, University of Vienna  
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 : Postdoc, 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

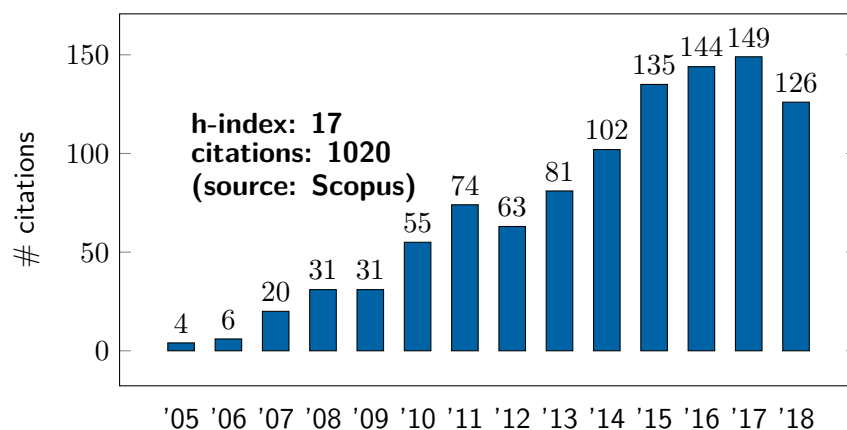
## Education

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>

## 10 most cited publications

- <sup>1</sup>P. Faccioli, M. Sega, F. Pederiva, and H. Orland, “Dominant pathways in protein folding”, *Phys. Rev. Lett.* **97**, 108101 (2006).
- <sup>2</sup>L. B. Pártay, P. Jedlovsky, M. Sega, L. B. Pártay, P. Jedlovsky, and M. Sega, “Molecular aggregates in aqueous solutions of bile acid salts. Molecular dynamics simulation study”, *J. Phys. Chem. B* **111**, 9886–9896 (2007).
- <sup>3</sup>L. B. Pártay, M. Sega, P. P. Jedlovsky, L. B. Pártay, M. Sega, and P. P. Jedlovsky, “Morphology of bile salt micelles as studied by computer simulation methods”, *Langmuir* **23**, 12322–12328 (2007).
- <sup>4</sup>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).
- <sup>5</sup>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).
- <sup>6</sup>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).
- <sup>7</sup>M. Sega, S. S. Kantorovich, P. Jedlovsky, and M. Jorge, “The generalized identification of truly interfacial molecules (ITIM) algorithm for nonplanar interfaces”, *J. Chem. Phys.* **138**, 044110 (2013).
- <sup>8</sup>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).
- <sup>9</sup>E. Autieri, P. Faccioli, M. Sega, F. Pederiva, and H. Orland, “Dominant reaction pathways in high-dimensional systems”, *J. Chem. Phys.* **130**, 064106 (2009).
- <sup>10</sup>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).