

# Riccardo Spezia

## CURRICULUM VITAE

### Adresse

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### Professional Preparation

2000 *Laurea* (M.S.) in Chemistry, Università di Roma « La Sapienza », Italy  
2004 Ph.D in Chemistry, Università di Roma « La Sapienza », Italy  
2004 – 2005 CNRS Postdoctoral Fellow, Ecole Normale Supérieure, Paris, France  
2005 – 2006 CNRS Postdoctoral Fellow, Université d'Evry-Val-d'Essonne, France  
2012 Habilitation (HDR), Université d'Evry-Val-d'Essonne, France

### Academic/Professional Appointments

2018 – ... CNRS Research Director (DR2) in Theoretical Chemistry, Laboratoire de Chimie Théorique (LCT), Sorbonne Université.  
2017 – 2018 Senior (CRCN) CNRS researcher at Laboratoire de Chimie Théorique (LCT), Sorbonne Université.  
2010 – 2018 Senior (CR1) CNRS researcher in Theoretical Chemistry, LAMBE, Université d'Evry-Val-d'Essonne.  
2006 – 2010 Junior (CR2) CNRS researcher in Theoretical Chemistry, LAMBE, Université d'Evry-Val-d'Essonne.

### Honors and Awards

2017 Invited professor at *Universidad de Valladolid*, Spain.  
2015 PEDR CNRS (Research and advising prize of CNRS).  
2015 – 2018 ANR “DynBioReact”: “*Development and Application of Direct Dynamics Simulations for Reactivity of Biological Molecules*”. International project with NSF. USA partner: Prof. W.L.Hase (Texas Tech University). ANR PI, funding: 330000€.  
2013 – 2015 Labex Charm3at project “*Détermination des mécanismes de dissociation induite par collision d’oligosaccharides en phase gazeuse par simulations de dynamique moléculaire*”. Funding: 50000€.  
2011 – 2014 ANR young researcher project (JCJC-2010) “*ACLASOLV*”: “*Solvatation d’actinides et lanthanides*”. Funding: 150000€.

## Publication record

110 papers in peer reviewed journals (times cited 2144, h-index 25).

The full list of publication is available here:

<http://www.lct.jussieu.fr/pagesperso/rspezia/pagine/pubblicazioni.html>

## Five Recent Publications Closely Related to the Project

- 1) K.Song and R.Spezia. *Theoretical Mass Spectrometry. Tracing ions with chemical trajectories*. De Gruyter, Berlin (2018). ISBN: 978-3-11-043489-7.
- 2) A.Martin-Somer, J.Martens, J.Grzetic, W.L.Hase, J.Oomens and R.Spezia. *Unimolecular Fragmentation of Deprotonated Diproline [Pro<sub>2</sub>-H]<sup>-</sup> Studied by Chemical Dynamics Simulations and IRMPD Spectroscopy*. J. Phys. Chem. A **122**, 2612-2625 (2018).
- 3) Z.Homayoon, V.Macaluso, A.Martin-Somer, M.C.N.Barbosa Muniz, I.Borges, Jr., W.L.Hase and R.Spezia. *Chemical Dynamics Simulations of Peptide Ion CID. Comparisons between TIK(H<sup>+</sup>)<sub>2</sub> and TLK(H<sup>+</sup>)<sub>2</sub> Fragmentation Dynamics, and with Thermal Simulations*. Phys. Chem. Chem. Phys. **20**, 3614-3629 (2018).
- 4) R.Spezia, A.Martin-Somer, V.Macaluso, Z.Homayoon, S.Pratihar and W.L.Hase. *Unimolecular Dissociation of Peptides: Statistical vs Non-Statistical Fragmentation Mechanisms and Time Scales*. Faraday Discuss. **195**, 599-618 (2016).
- 5) R.Spezia, J.Martens, J.Oomens and K.Song. *Collision-induced dissociation pathways of protonated Gly<sub>2</sub>NH<sub>2</sub> and Gly<sub>3</sub>NH<sub>2</sub> in the short time-scale limit by chemical dynamics and ion spectroscopy*. Int. J. Mass Spectrom. **388**, 40-52 (2015).

## Mentoring activities

PhD advisor and co-advisor of 7 students.

Advisor and co-advisor of 6 post-doctoral fellows.

Responsible of 16 undergraduate students (from L3 to M2).

## Synergistic Activities

- 2019 – ... Member of the board of Physical Chemistry Division of the *Société Chimique de France*. Elected as general secretary.
- 2018 – ... Head of the group “Dynamic simulations: structure and reactivity” at Laboratoire de Chimie Théorique, Sorbonne Université.
- 2015 – ... Member of the board of Ile-de-France section of the *Société Chimique de France*.
- 2015 – 2018 Member of direction committee of *the Fédération de recherche Chimie Physique de Paris Saclay* (FR 3510 CNRS).
- 2014 – 2018 Co-head of the group “Interactions in complex molecular assemblies: theory and simulations” at LAMBE, Université d’Evry-Val-d’Essonne.

## Principal Collaborations

William L. Hase (Texas Tech University, USA)

Kihyung Song (Korea National University of Education, Korea)

Paola D'Angelo, Enrico Bodo, Sergio Brutti (Università di Roma "La Sapienza", Italy)  
Debora Scuderi (Université Paris-Sud, France)  
Jean-Yves Salpin, Yannick Jeanvoine (Université d'Evry-Val-d'Essonne, France)  
Manuel Yanez (Universidad Autonoma de Madrid, Spain)  
Antonio Largo (Universidad de Valladolid, Spain)  
Rodolphe Vuilleumier (Ecole Normale Supérieure et Sorbonne Université, France)