Curriculum Vitae

Albert Rimola

June 2014

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PERSONAL DATA

Name: Albert RIMOLA

Date of birth: 22/07/1980

Place of birth: Barcelona

Nationality: Spanish

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ACADEMIC RECORD

2002: **DEGREE in CHEMISTRY**

Universitat Autònoma de Barcelona

Issue Date: 30/09/2002

2003: **MASTER in THEORETICAL AND COMPUTATIONAL CHEMISTRY**

Universitat Autònoma de Barcelona

Excellent with honours

Issue Date: 21/12/2003

2007: **PhD in THEORETICAL AND COMPUTATIONAL CHEMISTRY**

Universitat Autònoma de Barcelona

Title: **Activation of Amino Acids and Peptides by Interaction of Cu^{+} and Cu^{2+} and Aluminosilicates Surfaces**

Supervisors: **Prof. Mariona Sodupe** and **Dr. Luis Rodríguez-Santiago**

Qualification: **Excellent – *cum laude***

Issue Date: 08/03/2007

POSITIONS

Current Position

- **DISTINGUISHED POSTDOCTORAL RESEARCHER**

  Dep. Chemistry of Universitat Autònoma de Barcelona (UAB).

  (01/10/2014 to present)

Previous Positions

- **COLLABORATION GRANT**
  Dep. Chemistry of UAB.
  (01/10/2002 – 31/12/2002)

- **UAB PREDOCTORAL RESEARCH FELLOW**
  Dep. Chemistry of UAB.
  (01/01/2003 – 14/09/2006)

- **1-YEAR TEACHING ASSISTANT CONTRACT**
  Dep. Chemistry of UAB.
  (15/09/2006 – 14/09/2007)

- **RAMÓN ARECES POSTDOCTORAL RESEARCH FELLOW**
  Dep. Chemistry IFM of University of Turin.
  (01/10/2007 – 30/11/2009)

- **UAB POSTDOCTORAL RESEARCH CONTRACT**
  Dep. Chemistry of UAB.
  (01/12/2009 – 31/03/2010)

- **BEATRIU DE PINÓS POSTDOCTORAL RESEARCH CONTRACT**
  Dep. Chemistry of UAB.
  (01/04/2010 – 30/09/2011)

- **JUAN DE LA CIERVA POSTODCTORAL RESEARCH CONTRACT**

  Dep. Chemistry of UAB.

  (01/10/2011 – 30/09/2014)

VISITS TO FOREIGN RESEARCH CENTERS

- **UNIVERSITY of ÉVRY – VAL D'ESSONNE** (France)
  Supervisor: Prof. Jeanine TORTAJADA
  Predoctoral visit
  (23/04/2004 – 22/07/2004)

- **UNIVERSITY of TURIN** (Italy)
  Supervisor: Prof. Piero UGLIENGO
  Predoctoral visit
  (26/04/2005 – 22/07/2005)

- **UNIVERSITY of KENT** (United Kingdom)
  Supervisor: Prof. Philip LINDAN
  Predoctoral visit
  (02/04/2006 – 01/05/2006)

- **UNIVERSITY of TURIN** (Italy)
  Supervisor: Prof. Piero UGLIENGO
  Postdoctoral work
  (01/10/2007 – 30/11/2009)

FUNDING ID RESEARCH PROJECTS

As Principal Investigator

1. PROJECT TITLE: "In silico prediction of the physico-chemical features of silicate interstellar dust" (CTQ2013-40347-ERC)
   FUNDING AGENCY: MINECO (Spanish Government)
   AMOUNT: 59,800 €
   PERIOD: December 2013 – February 2015

2. PROJECT TITLE: "Quantum chemical studies of electronic structure and chemical reactivity of dust nanoparticles of astrochemical interest" (CTQ2014-60119-P)
   FUNDING AGENCY: MINECO (Spanish Government)
   AMOUNT: 45,000 €
   PERIOD: July 2015 – June 2017

As Participant

1. PROJECT TITLE: "Group of structure and chemical reactivity" (2001SGR-00812)
   PRINCIPAL INVESTIGATOR: Prof. Juan Bertrán
   FUNDING AGENCY: DGR (Catalan Government)
   PERIOD: 2001 – 2004

2. PROJECT TITLE: "Ionisation and activation of systems with biochemical interest by metal cations. Mass spectrometry and theoretical studies" (BQU2002-04112-C02-01)
   PRINCIPAL INVESTIGATOR: Prof. Mariona Sodupe
   FUNDING AGENCY: MCyT (Spanish Government)
   PERIOD: 2003 – 2005

3. PROJECT TITLE: "Group of theoretical studies on biomolecule activation" (2005-SGR-00244)
   PRINCIPAL INVESTIGATOR: Prof. Mariona Sodupe
   FUNDING AGENCY: DURSI (Catalan Government)
   PERIOD: 2005 – 2008

4. PROJECT TITLE: "Activation of biomolecules. Computational and mass spectrometry studies" (CTQ2005-08797-C02-02/BQU)
   PRINCIPAL INVESTIGATOR: Prof. Mariona Sodupe
   FUNDING AGENCY: MEC (Spanish Government)
   PERIOD: 2006 – 2008

5. PROJECT TITLE: "Interface phenomena in silica-based nanostructured biocompatible materials contacted with biological systems" (COFIN2006, Prot. 200632335_005)
   PRINCIPAL INVESTIGATOR: Prof. Claudio Morterra
   FUNDING AGENCY: MIUR (Italian Government)
   PERIOD: 2007 – 2009

6. PROJECT TITLE: "Activation of biomolecules by metal cations and silica-based surfaces" (CTQ2008-06381/BQU)
   PRINCIPAL INVESTIGATOR: Prof. Mariona Sodupe
   FUNDING AGENCY: MICINN (Spanish Government)
   PERIOD: 2009 – 2011

7. PROJECT TITLE: "Group of theoretical studies on biomolecule activation" (2008-SGR-638)
   PRINCIPAL INVESTIGATOR: Prof. Mariona Sodupe
   FUNDING AGENCY: DURSI (Catalan Government)
   PERIOD: 2009 – 2013

8. PROJECT TITLE: "Computational studies of structure and chemical reactivity. Application to systems of biological interest" (CTQ2011-24847)
   PRINCIPAL INVESTIGATOR: Prof. Mariona Sodupe
   FUNDING AGENCY: MICINN (Spanish Government)
   PERIOD: 2011 – 2013

9. PROJECT TITLE: "Bioinorganic computational group" (2014-SGR-482)
   PRINCIPAL INVESTIGATOR: Prof. Mariona Sodupe
   FUNDING AGENCY: DURSI (Catalan Government)
   PERIOD: 2014 – 2018

Summary

- **50 PUBLICATIONS** in internationally peer-reviewed journals
- **1 BOOK CHAPTER**
- **SCOPUS INDICATORS:** h-index = 20
  1005 citations (890 without self-citations)
  Average citation per item = 20.1
- **10 INVITED PRESENTATIONS**
- **1 PhD SUPERVISION** (in progress)
- **2 end-of-degree research work SUPERVISION** (in progress)
- **1 Postdoc SUPERVISION**

Overview

The focus of the research of Dr. A. Rimola has always been on modeling chemical processes by accurate quantum chemical calculations using both molecular and periodic ab-initio approaches.

His PhD was devoted to the metal-ion gas phase chemistry, in which quantum chemical calculations were essential to interpret the complex outcome of mass spectrometry experiments. During this period he acquired a very good knowledge of different quantum mechanical methods for the treatment of open-shell systems and gained experience in the simulation of chemical reactivity.

During his post-doc, Dr. A. Rimola studied the electronic structure of different solid-state extended systems and of their adsorptive and chemical reactivity properties, getting deep experience in the modeling of surfaces of different nature; *e.g.*, ionic/covalent, crystalline/amorphous, defective, etc.

The expertise of Dr. A. Rimola is thus on the simulation of chemical reactivity and modeling of complex surfaces and his current research activity merges and exploits these two skills, which are of great interest in several fields like heterogeneous catalysis, surface science, nanostructures and biomaterials.

His current research lines focus on the modeling of processes of astrochemical and prebiotic interest in which solid state systems (namely, cosmic dust, dirty ices and natural minerals) play an important role.

He holds several international collaborations with quantum chemists (Prof. P. Ugliengo, Univ. Turin; Prof. A. Michealides, Univ. College London), experimentalists (Prof. T. Chiavassa, Univ. Marseille; Prof. J.-F. Lambert, Univ. Pierre et Marie Curie, Prof. G. Martra, Univ. Turin)

and astronomers (Prof. C. Ceccarelli, Grenoble Observatory; Prof. J. Cernicharo, ICMM-CSIC; Dr. J.M. Trigo-Rodríguez (ICE-CSIC).

Articles

1. Javier Navarro-Ruiz, José Ángel Martínez-González, Mariona Sodupe, Piero Ugliengo, Albert Rimola*. "Relevance of silicate surface morphology in interstellar H_2 formation. Insights from quantum chemical calculations". *Monthly Notices of the Royal Astronomical Society*, **2015**, Accepted.

2. Albert Rimola*. "Intrinsic Ladders of Affinity for Amino Acid-Analogues on Boron Nitride Nanomaterials. A B3LYP-D2* Periodic Study". *Journal of Physical Chemistry C*, **2015**, Accepted, DOI: 10.1021/acs.jpcc.5b04601

3. Aurélien Fresneau, Gregoire Danger, Albert Rimola, Fabrice Duvernay, Patrice Theulé, Thierry Chiavassa. "Ice chemistry of acetaldehyde reveals competitive reactions in the first step of Strecker synthesis of alanine: formation of HO-CH(CH_3)-NH_2 vs. HO-CH(CH_3)-CN". *Monthly Notices of the Royal Astronomical Society*, **2015**, 451, 1649-1660.

4. Albert Rimola*, Vianney Taquet, Piero Ugliengo, Nadia Balucani, Cecilia Ceccarelli. "Combined quantum chemical and modeling study of CO hydrogenation on water ice". *Astronomy & Astrophysics*, **2014**, 572, A70.

5. Fabrice Duvernay, Albert Rimola*, Patrice Theulé, Gregoire Danger, T. Sanchez, Thierry Chiavassa. "Formaldehyde chemistry in cometary ices: the case of $HOCH_2OH$ formation". *Physical Chemistry Chemical Physics*, **2014**, 16, 24200- 24208.

6. Aurélien Fresneau, Grégoire Danger, Albert Rimola, Patrice Theulé, Fabrice Duvernay, Thierry Chiavassa. "Trapping in water – an important prerequisite for complex reactivity in astrophysical ices: the case of acetone $(CH_3)_2C=O$ and ammonia NH_3. *Monthly Notices of the Royal Astronomical Society*, **2014**, 443, 2991-3000.

7. Fabrice Duvernay, Gregoire Danger, Patrice Theulé, Thierry Chiavassa, Albert Rimola*. "Formaldehyde chemistry in cometary ices: on the prospective detection of NH_2CH_2OH, $HOCH_2OH$, and POM by the on-board ROSINA instrument of the Rosetta mission". *Astrophysical Journal*, **2014**, 791, 75.

8. Albert Rimola*, Mariona Sodupe. "Gas-Phase and Microsolvated Glycine Interacting with Boron Nitride Nanotubes. A B3LYP-D2* Periodic Study". *Inorganics*, **2014**, 2, 334-350.

9. Javier Navarro-Ruiz, Mariona Sodupe, Piero Ugliengo, Albert Rimola*. "Interstellar H adsorption and H_2 formation on the crystalline (010) forsterite surface: a B3LYP-D2* periodic study". *Physical Chemistry Chemical Physics*, **2014**, 16, 17447-17457.

10. Javier Navarro-Ruiz, Piero Ugliengo, Albert Rimola*, Mariona Sodupe. "B3LYP Periodic Study of the Physicochemical Properties of the Nonpolar (010) Mg-Pure and Fe-Containing Olivine Surfaces". *J. Phys. Chem. A*, **2014**, 118, 5866-5875.

11. Gregoire Danger, Albert Rimola*, Ninette Abou Mrad, Fabrice Duvernay, Gaël Roussin, Patrice Theulé, Thierry Chiavassa. "Formation of hydroxyacetonitrile ($HOCH_2CN$) and polyoxymethylene (POM)-derivatives in comets from formaldehyde (CH_2O) and hydrogen cyanide (HCN) activated by water". *Physical Chemistry Chemical Physics*, **2014**, 16, 3360-3370.

12. Javier Navarro-Ruiz, Albert Rimola*, Mariona Sodupe. "Surface Reaction of Acetylene with H-terminated Silicon Surfaces. A Theoretical Study from Hybrid DFT-D2 Periodic Simulations". *Journal of Physical Chemistry C*, **2013**, 117, 15130-15138.

13. Albert Rimola*, Mariona Sodupe. "Physisorption *vs* Chemisorption of Probe Molecules on Boron Nitride Nanomaterials. Effect of Surface Curvature". *Physical Chemistry Chemical Physics*, **2013**, 15, 13190-13198.

14. Albert Rimola, Dominique Costa, Mariona Sodupe, Jean François Lambert, Piero Ugliengo. "Silica surface features and their role in the adsorption of bio-molecules: computational modeling and experiments". *Chemical Reviews*, **2013**, 113, 4216-4313.

15. Jorge Alí-Torres, Albert Rimola, Cristina Rodríguez-Rodríguez, Luis Rodríguez-Santiago, Mariona Sodupe. "Insights on the Binding of Thioflavin Derivative Markers to Amyloid-Like Fibril Models From Quantum Chemical Calculations". *Journal of Physical Chemistry B*, **2013**, 117, 6674-6680.

16. Vassilissa Vinogradoff, Albert Rimola*, Fabrice Duvernay, Gregoire Danger, Patrice Theulé, and Thierry Chiavassa. "The mechanism of hexamethylenetetramine (HMT) formation in the solid state at low temperature". *Physical Chemistry Chemical Physics*, **2012**, *14*, 12309-12320.

17. Albert Rimola*, Mariona Sodupe, Piero Ugliengo. "Computational Study of Interstellar Glycine Formation Occurring at Radical Surfaces of Water-Ice Dust Particles". *The Astrophysical Journal*, **2012**, *754*, 24.

18. Elisa Jimenez-Izal, Fabio Chiatti, Marta Corno, Albert Rimola, Piero Ugliengo. "Glycine Adsorption at Nonstoichiometric (010) Hydroxyapatite Surfaces: A B3LYP Study". *Journal of Physical Chemistry C*, **2012**, *116*, 14561-14567.

19. Albert Rimola, Massimiliano Aschi, Roberto Orlando, Piero Ugliengo. "Does Adsorption at Hydroxyapatite Surfaces Induce Peptide Folding? Insights from Large-Scale B3LYP Calculations". *Journal of the American Chemical Society*, **2012**, *134*, 10899-10910.

20. Albert Rimola, Marta Corno, Jorge Garza, Piero Ugliengo. "Ab initio modelling of protein–biomaterial interactions: influence of amino acid polar side chains on

adsorption at hydroxyapatite surfaces". *Philosophical Transactions of the Royal Society A*, **2012**, *370*, 1478-1498.

21. Albert Rimola, Jorge Alí-Torres, Cristina Rodríguez-Rodríguez, Jordi Poater, Eduard Matito, Miquel Solà, Mariona Sodupe. "Ab Initio Design of Chelating Ligands Relevant to Alzheimer's Disease: Influence of Metalloaromaticity". *Journal of Physical Chemistry A*, **2011**, *115*, 12659–12666.

22. Albert Rimola, Yuriy Sakhno, Luca Bertinetti, Marco Lelli, Gianmario Martra, Piero Ugliengo. "Toward a Surface Science Model for Biology: Glycine Adsorption on Nanohydroxyapatite with Well-Defined Surfaces". *The Journal of Physical Chemistry Letters*, **2011**, *2*, 1390-1394.

23. Piero Ugliengo, Albert Rimola, Mariona Sodupe. "In silico study of the interstellar prebiotic formation and delivery of glycine". *Rendiconti Lincei – Scienze Fisiche e Naturali*, **2011**, *22*, 137-144.

24. Cristina Rodríguez-Rodríguez, Albert Rimola, Jorge Alí-Torres, Mariona Sodupe, Pilar González-Duarte. "In silico strategies for the selection of chelating compounds with potential application in metal-promoted neurodegenerative deseases". *Journal of Computer-Aided Molecular Design*, **2011**, *25*, 21-30.

25. Marta Corno, Albert Rimola, Vera Bolis, Piero Ugliengo. "Hydroxyapatite as a key biomaterial: quantum-mechanical simulation of its surfaces in interaction with bio-molecules". *Physical Chemistry Chemical Physics*, **2010**, *12*, 6309-6329.

26. Albert Rimola, Bartolomeo Civalleri, Piero Ugliengo. "Physisorption of aromatic organic contaminants at the surface of hydrophobic/hydrophilic silica geosorbents: a B3LYP-D modeling study". *Physical Chemistry Chemical Physics*, **2010**, *12*, 6357-6366.

27. Albert Rimola, Claudio Zicovich-Wilson, Roberto Dovesi, Piero Ugliengo. "Search and Characterization of Transition State Structures in Crystalline Systems using Valence Coordinates". *Journal of Chemical Theory and Computation*, **2010**, *6*, 1341-1350.

28. Albert Rimola, Mariona Sodupe, Piero Ugliengo. "Deep-space glycine formation via Strecker-type reactions activated by ice water dust mantles. A computational approach". *Physical Chemistry Chemical Physics*, **2010**, *12*, 5285-5294.

29. Cristina Rodríguez-Rodríguez, Albert Rimola, Luis Rodríguez-Santiago, Piero Ugliengo, Ángel Álvarez-Larena, Hugo Gutiérrez-de-Terán, Mariona Sodupe, Pilar González-Duarte. "Crystal structure of thioflavin-T and its binding to amyloid fibrils: insights at the molecular level". *Chemical Communications*, **2010**, *46*, 1156-1158.

30. Albert Rimola, Marta Corno, Claudio Zicovich-Wilson, Piero Ugliengo. "Ab initio modeling of protein/biomaterial interactions: competitive adsorption between glycine and water onto hydroxyapatite surfaces". *Physical Chemistry Chemical Physics*, **2009**, *11*, 9005-9007.

31. Erika Constantino, Albert Rimola, Mariona Sodupe, Luis Rodríguez-Santiago. "Coordination of (Glycyl)nglycine (n= 1-3) to Co^{+} and Co^{2+}". *Journal of Physical Chemistry A*, **2009**, *113*, 8883-8892.

32. Albert Rimola, Mariona Sodupe, Piero Ugliengo. "Affinity scale for the interaction of amino acids with silica surfaces". *Journal of Physical Chemistry C*, **2009**, *113*, 5741-5750.

33. Albert Rimola, Piero Ugliengo, Mariona Sodupe. "Formation versus hydrolysis of the peptide bond from a quantum-mechanical viewpoint: the role of mineral surfaces and implications for the origin of life". *International Journal of Molecular Sciences*, **2009**, *10*, 746-760 (Special Issue "Origin of Life").

34. Albert Rimola, Piero Ugliengo. "The role of defective silica surfaces in exogenous delivery of prebiotic compounds: clues from first principles calculations". *Physical Chemistry Chemical Physics*, **2009**, *11*, 2497-2506.

35. Cristina Rodríguez-Rodríguez, Natalia de Groot, Albert Rimola, Angel Alvarez-Larena, Vega Lloveras, José Vidal-Gancedo, Salvador Ventura, Josep Vendrell, Mariona Sodupe, Pilar González-Duarte, Pilar. "Design, selection and characterization of thioflavin-based intercalation compounds with metal chelating properties for application in Alzheimer's disease". *Journal of the American Chemical Society*, **2009**, *131*, 1436-1451.

36. Albert Rimola, Marta Corno, Claudio Zicovich-Wilson, Piero Ugliengo. "Ab initio modeling of protein/biomaterial interactions: glycine adsorption at hydroxyapatite surfaces". *Journal of the American Chemical Society*, **2008**, *130*, 16181-16183.

37. Albert Rimola, Bartolomeo Civalleri, Piero Ugliengo. "Neutral vs zwitterionic glycine forms at the water/silica interface: structure, energies, and vibrational features from B3LYP periodic simulations". *Langmuir*, **2008**, *24*, 14027-14034.

38. Albert Rimola, Piero Ugliengo. "A quantum mechanical study of the reactivity of $(SiO)_2$-defective silica surfaces". *Journal of Chemical Physics*, **2008**, *128*, 204702.

39. Albert Rimola, Erika Constantino, Luis Rodríguez-Santiago, Mariona Sodupe. "Binding properties of $Cu^{+/2+}$-(glycyl)nglycine complexes (n= 1–3)". *Journal of Physical Chemistry A*, **2008**, *112*, 3444-3453.

40. Albert Rimola, Mariona Sodupe, Piero Ugliengo. "Aluminosilicate surfaces as promoters for peptide bond formation: an assessement of Bernal's hypothesis by ab-initio methods". *Journal of the American Chemical Society*, **2007**, *129*, 8333-8344.

41. Albert Rimola, Luis Rodríguez-Santiago, Piero Ugliengo, Mariona Sodupe. "Is the peptide bond formation activated by Cu^{2+} interactions? Insights from first principles calculations". *Journal of Physical Chemistry B*, **2007**, *111*, 5740-5747.

42. Albert Rimola, Luis Rodríguez-Santiago, Mariona Sodupe. "Relevance of cation-π interactions and oxidative effects on Cu^{+} and Cu^{2+} binding to Phe, Tyr, Trp and His. New insights from first-principles calculations". *Journal of Physical Chemistry B*, **2006**, *110*, 24189-24199.

43. Albert Rimola, Mariona Sodupe, Jeanine Tortajada, Luis Rodriguez-Santiago. "Gas phase reactivity of Cu^{+}-aromatic amino acids. An experimental and theoretical study". *International Journal of Mass Spectrometry*, **2006**, *257*, 60-69.

44. Albert Rimola, Mariona Sodupe, Sergio Tosoni, Bartolomeo Civalleri, Piero Ugliengo. "Interaction of glycine with isolated hydroxyl groups at the silica surface: first principles B3LYP periodic simulation". *Langmuir*, **2006**, *22*, 6593-6604.

45. Mar Tristany, James Courmarcel, Philippe Dieudonné, Marcial Moreno-Mañas, Roser Pleixats, Albert Rimola, Mariona Sodupe, Silvia Villarroya. "Palladium nanoparticles entrapped in heavily fluorinated compounds". *Chemistry of Materials*, **2006**, *18*, 716-722.

46. Albert Rimola, Mariona Sodupe, Josep Ros, Josefina Pons. "A theoretical study on Pd^{II} complexes containing hemilabile pyrazole-derived ligands". *European Journal of Inorganic Chemistry*, **2006**, 447-454.

47. Albert Rimola, Sergio Tosoni, Mariona Sodupe, Piero Ugliengo. "Does silica surface catalyze peptide bond formation? New insights from first-principles calculations". *ChemPhysChem*, **2006**, *7*, 157-163.

48. Erika Constantino, Albert Rimola, Luis Rodríguez-Santiago, Mariona Sodupe. "Coordination properties of Glycylglycine to Cu^{+}, Ni^{+} and Co^{+}. Influence of metal cation electronic configuration". *New Journal of Chemistry*, **2005**, *29*, 1585-1593.

49. Albert Rimola, Sergio Tosoni, Mariona Sodupe, Piero Ugliengo. "Peptide bond formation activated by the interplay of Lewis and Brønsted catalysts". *Chemical Physics Letters*, **2005**, *408*, 295-301.

50. Jordi Poater, Miquel Solà, Albert Rimola, Luis Rodríguez-Santiago, Mariona Sodupe. "Ground and low-lying states of Cu^{2+}-H_2O. A difficult case for density functional methods". *Journal of Physical Chemistry A*, **2004**, *108*, 6072-6078.

Book Chapters

1. Albert Rimola, Mariona Sodupe, Piero Ugliengo. "Computational simulations of prebiotic processes", pp 345-362. In *Genesis: Origin of Life on Earth and Planets* (Editor: Joseph Seckbach), Springer Netherlands, 2012.

Invited Conferences

1. TITLE: “Contribution of Quantum Chemical Methods in the Study of Ice-Based Cosmochemistry”
   CONGRESS: *Second Workshop on Experimental Laboratory Astrophysics*
   PLACE and YEAR: Poipu, Kauai, Hawaii (USA), 2015

2. TITLE: “Atomic-Scale Insights of the Chemistry Occurring in the Interstellar Medium. Clues from Quantum Chemical Mathods”
   CONGRESS: *Workshop on Interstellar Matter 2014*
   PLACE and YEAR: Sapporo (Japan), 2014

3. TITLE: “Computational Study on the Formation of H_2 and CH_3OH on Surfaces of Interstellar Dust Particles”
   CONGRESS: *World Association of Theoretical and Computational Chemists* (WATOC 2014)
   PLACE and YEAR: Santiago de Chile (Chile), 2014

4. TITLE: “Computational Study of Alkyne Reactions with Hydrogenated Silicon Surfaces. Free Energy Effects on Competitive Processes”
   CONGRESS: *10th International Conference of Computational Methods in Sciences and Engineering*
   PLACE and YEAR: Athens (Greece), 2014

5. TITLE: “Theoretical studies on the abiotic formation of biomolecules on inorganic surfaces”
   CONGRESS: *Biomolecules on surfaces: from abiotic polymerization to biosensors*
   PLACE and YEAR: Turin (Italy), 2014

6. TITLE: “Contribution of Quantum Mechanical Calculations in the Cosmic Dust Chemical Studies”
   CONGRESS: *Evolution of the Organic Matter in the Heart of the Interstellar and Interplanetary Medium*
   PLACE and YEAR: Paris (France), 2013

7. TITLE: “Interstellar Formation of Glycine on Radical Surfaces of Water Ice Particles”
   CONGRESS: *Theoretical Computational Astrochemistry*
   PLACE and YEAR: Pisa (Italy), 2012

8. TITLE: “Quantum Chemical Simulations on Interstellar Synthesis of Glycine: Neutral vs Radical Cation Mechanisms on Water Ice Dust Particles”
   CONGRESS: *Challenges in Modelling the Reaction Chemistry of Interstellar Dust*
   PLACE and YEAR: Leiden (Netherlands), 2011

9. TITLE: “Transition State Search with CRYSTAL09”

CONGRESS: *Ab Initio Modeling in Solid State Chemistry 2009* (International Advanced School)
PLACE and YEAR: Turin (Italy), 2009

10. TITLE: "Amino Acid Synthesis on Icy Interstellar Particles. Computational Modeling Studies"
    CONGRESS: *Prebiotic Chemistry* (International Advanced School)
    PLACE and YEAR: Barcelona (Spain), 2008

Oral Communications

1. TITLE: "Quantum Mechanical Contributions in the Study of Ice-Based Astrochemical Problems"
   CONGRESS: *COST Action Our Astrochemical History CM1401 – First General Meeting*
   PLACE and YEAR: Prague (Czech Republic), 2015

2. TITLE: "Formation of H_2CO on Icy Water Dust Particles from a Computational Approach: Polarizing and Electron Charge Effects"
   CONGRESS: *Origins 2014*
   PLACE and YEAR: Nara (Japan), 2014

3. TITLE: "Polarizing and Electrons Charge Effects for the Formation of CH2O on Surfaces of Water Icy Dust Particles"
   CONGRESS: *247th American Chemical Society National Meeting & Exposition*
   PLACE and YEAR: Dallas (USA), 2014

4. TITLE: "Naturally Occurring Mineral Surface Defects. A Meeting Point between Industrial and Prebiotic Chemistry"
   CONGRESS: *7th Congress on Electronic Structure: Principles and Applications* (ESPA2010)
   PLACE and YEAR: Oviedo (Spain), 2010

5. TITLE: "Peptide Bond Formation Mediated by Cu^{2+}. Insights from First Principles Calculations"
   CONGRESS: *23rd Meeting of the Theoretical and Computational Chemistry Reference Network*
   PLACE and YEAR: Tarragona (Spain), 2007

6. TITLE: "Role of Aluminosilicates on Peptide Bond Formation. A Theoretical Mechanistic Study"
   CONGRESS: *4th Meeting of the Young Researchers of the Catalan Countries*
   PLACE and YEAR: Lleida (Spain), 2006

Posters

1. AUTHORS: Albert Rimola, Josep M. Trigo-Rodríguez, Zita Martins,
   TITLE: "Processing of primordial organic compounds in carbonaceous asteroids by mild aqueous alteration"
   CONGRESS: *Asteroid Day 2015*
   PLACE and YEAR: Barcelona (Spain), 2015

2. AUTHORS: Albert Rimola, Josep M. Trigo-Rodríguez, Zita Martins, Carles E. Moyano-Cambero
   TITLE: "Processing of primordial organic compounds in carbonaceous asteroids by mild aqueous alteration"
   CONGRESS: *Origins 2014*
   PLACE and YEAR: Nara (Japan), 2014

3. AUTHORS: Albert Rimola, Javier Navarro-Ruiz, Mariona Sodupe, Piero Ugliengo
   TITLE: "Quantum mechanical insights into molecular hydrogen formation on interstellar dust grains"
   CONGRESS: *Origins 2014*
   PLACE and YEAR: Nara (Japan), 2014

4. AUTHORS: Albert Rimola, Javier Navarro-Ruiz, Mariona Sodupe, Piero Ugliengo
   TITLE: "Quantum mechanical insights into molecular hydrogen formation on interstellar dust grains"
   CONGRESS: *Astrochemistry of Ice, Dust and Gas (Faraday Discussion 168)*
   PLACE and YEAR: Leiden (Nederlands), 2014

5. AUTHORS: Albert Rimola, Mariona Sodupe, Piero Ugliengo
   TITLE: "Interstellar formation of glycine on radical surfaces of water ice particles"
   CONGRESS: *8th Congress on Electronic Structure: Principles and Applications* (ESPA2012)
   PLACE and YEAR: Barcelona (Spain), 2012

6. AUTHORS: Albert Rimola, Mariona Sodupe, Piero Ugliengo
   TITLE: "Glycine formation occurring at surfaces of radical cation ice water in the interstellar medium"
   CONGRESS: *World Association of Theoretical and Computational Chemists* (WATOC 2011)
   PLACE and YEAR: Santiago de Compostela (Spain), 2011

7. AUTHORS: Albert Rimola, Mariona Sodupe, Piero Ugliengo
   TITLE: "Interstellar glycine formation occurring at surfaces of ice water dust grain particles under ionizing effects"
   CONGRESS: *Origins 2011*
   PLACE and YEAR: Montpellier (France), 2011

8. AUTHORS: Albert Rimola, Mariona Sodupe
   TITLE: "Computational simulations of the interaction of boron nitride nanotubes with biomolecules. Insights on the nature of interaction"
   CONGRESS: *NANOJASP'2010: Nanomaterials based biosensors and biosystems*
   PLACE and YEAR: Barcelona (Spain), 2010

9. AUTHORS: Albert Rimola, Mariona Sodupe, Piero Ugliengo
   TITLE: "Deep-space glycine formation via Strecker-type reactions activated by ice water dust mantles. A computational approach"
   CONGRESS: *First chemical steps towards the origin of life*
   PLACE and YEAR: Turin (Italy), 2010

10. AUTHORS: Albert Rimola, Mariona Sodupe, Piero Ugliengo
    TITLE: "Interaction of amino acids with silica-based materials. New insights from DFT calculations"
    CONGRESS: *2nd European Chemistry Congress* (EuCheMS 2008)
    PLACE and YEAR: Turin (Italy), 2008

11. AUTHORS: Albert Rimola, Mariona Sodupe, Piero Ugliengo
    TITLE: "Prebiotic amino acid synthesis on crystalline icy particles. A computational approach"
    CONGRESS: *2nd European Chemistry Congress* (EuCheMS 2008)
    PLACE and YEAR: Turin (Italy), 2008

12. AUTHORS: Albert Rimola, Mariona Sodupe, Piero Ugliengo
    TITLE: "Interaction of amino acids with silica-based materials. New insights from DFT calculations"
    CONGRESS: *Ab initio simulation of crystalline solids: history and prospects* (Workshop in honour of Prof. Cesare Pisani)
    PLACE and YEAR: Turin (Italy), 2008

13. AUTHORS: Albert Rimola, Mariona Sodupe, Piero Ugliengo
    TITLE: "Prebiotic amino acid synthesis on crystalline icy particles. A computational approach"
    CONGRESS: *Ab initio simulation of crystalline solids: history and prospects* (Workshop in honour of Prof. Cesare Pisani)
    PLACE and YEAR: Turin (Italy), 2008

14. AUTHORS: Albert Rimola, Mariona Sodupe, Piero Ugliengo
    TITLE: "Prebiotic amino acid synthesis on water ice mantle-grains. A computational approach"
    CONGRESS: *XV International Conference on the Origin of Life* (ISSOL 2008)
    PLACE and YEAR: Florence (Italy), 2008

15. AUTHORS: Albert Rimola, Mariona Sodupe, Piero Ugliengo
    TITLE: "Affinity scale for the interaction of amino acids with silica surfaces"

CONGRESS: *12th International Conference on the Applications of Density Functional Theory* (DFT'07)
PLACE and YEAR: Amsterdam (Netherlands), 2007

16. AUTHORS: Albert Rimola, Mariona Sodupe, Piero Ugliengo
TITLE: "Hydrogen-bond and dispersion: the driving forces of the adsorption of amino acids on silica surfaces"
CONGRESS: *Modelling the Interaction of Biomolecules with Inorganic Surfaces*
PLACE and YEAR: Lyon (France), 2007

17. AUTHORS: Albert Rimola, Mariona Sodupe, Piero Ugliengo
TITLE: "Does glycine molecule interact with silica surface? A theoretical study using periodic methods"
CONGRESS: *11th International Conference on Theoretical Aspects of Catalysis* (ICTAC-11)
PLACE and YEAR: Berlin (Germany), 2006

18. AUTHORS: Albert Rimola, Mariona Sodupe, Jeanine Tortajada, Luis Rodríguez-Santiago
TITLE: "Réactivité en phase gazeuse du complexe [Cu His]$^+$: une étude expérimentale et théorique"
CONGRESS: *1er Symposium de Chimie et Biologie Analytiques: de la molécula au protéme* (SCBA 2005)
PLACE and YEAR: Montpellier (France), 2005

19. AUTHORS: Albert Rimola, Luis Rodríguez-Santiago, Mariona Sodupe, Sergio Tosoni, Piero Ugliengo
TITLE: "Role of Lewis sites in aluminosilicates on peptide bond formation. A theoretical mechanistic study"
CONGRESS: *12th International Symposium on Relation between Homogeneous and Heterogeneous Catalysis* (ISHHC-XII)
PLACE and YEAR: Florence (Italy), 2005

20. AUTHORS: Albert Rimola, Mariona Sodupe, Josefina Ponsa, Josep Ros
TITLE: "Searching the Best Tioether-Pyrazole Hemilabile Ligand in Pd (II) Complexes"
CONGRESS: *Computational Modelling of Catalysis* (CMC)
PLACE and YEAR: Müllheim an der Ruhr (Germany), 2003

Invited Seminars

1. TITLE: "Hints on the evolution of the molecular complexity in space from quantum mechanical simulations"
PLACE and YEAR: University of Marseille (Marseille, France), 2015

2. TITLE: "Quantum mechanical calculations to understand ice-based interstellar reactions. Atomistic interpretations and predictions"

PLACE and YEAR: Institute of Low Temperature Science of Hokkaido (ILTS) (Sapporo, Japan), 2014

3. TITLE: "Contribution of quantum chemistry in astrochemical studies"
   PLACE and YEAR: Institute of Space Sciences (ICE-CSIC) (Bellaterra, Spain), 2014

4. TITLE: "Quantum chemical simulations of cosmic dust-based interstellar reactions"
   PLACE and YEAR: University of Barcelona (Barcelona, Spain), 2013

5. TITLE: "Interaction and reactivity of biomolecules on inorganic materials"
   PLACE and YEAR: MATGAS 2000 AIE (Bellaterra, Spain), 2009

6. TITLE: "Ab initio modeling of protein/biomaterial interactions"
   PLACE and YEAR: University of Turin (Italy), 2008

7. TITLE: "Searching Transition States with the CRYSTAL code: a glance at the first attempts"
   PLACE and YEAR: University of Turin (Italy), 2008

Participation of my students in international congresses

1. TYPE OF PRESENTATION: Poster
   AUTHORS: Javier Navarro-Ruiz, Albert Rimola, Mariona Sodupe, Piero Ugliengo
   TITLE: "Interstellar H_2 formation on crystalline silicate surfaces"
   CONGRESS: *41st Congress of Theoretical Chemists of Latin Expression* (CHITEL 2015)
   PLACE and YEAR: Turin (Italy), 2015

2. TYPE OF PRESENTATION: Poster
   AUTHORS: José Ángel Martínez-González, Albert Rimola
   TITLE: "Electronic structure characterization of forsterite"
   CONGRESS: *9th Congress on Electronic Structure: Principles and Applications* (ESPA2014)
   PLACE and YEAR: Badajoz (Spain), 2014

3. TYPE OF PRESENTATION: Poster
   AUTHORS: Javier Navarro-Ruiz, Albert Rimola, Mariona Sodupe, Angelos Michaelides
   TITLE: "Dynamic effects in the diffusion of atomic H on interstellar silicate surfaces"
   CONGRESS: *16th workshop on dynamical phenomena at surfaces*
   PLACE and YEAR: Madrid (Spain), 2013

4. TYPE OF PRESENTATION: Oral Communication
   AUTHORS: Javier Navarro-Ruiz, Albert Rimola, Mariona Sodupe
   TITLE: "Computational study on alkyne reactivity on hydrogenated silicon surfaces"

CONGRESS: *8th meeting of youth researchers of Catalonia*
PLACE and YEAR: Andorra la Vella (Andorra), 2013

5. TYPE OF PRESENTATION: Oral Communication
   AUTHORS: Javier Navarro-Ruiz, Albert Rimola, Mariona Sodupe
   TITLE: "H_2 formation on surfaces of interstellar dust"
   CONGRESS: *29th Annual meeting of the reference network of theoretical and computational chemistry of Catalonia*
   PLACE and YEAR: Barcelona (Spain), 2013

6. TYPE OF PRESENTATION: Oral Communication
   AUTHORS: Javier Navarro-Ruiz, Albert Rimola, Mariona Sodupe
   TITLE: "Ab initio insights into H_2 formation on interstellar dust grains"
   CONGRESS: *39th International Congress of Theoretical Chemists of Latin Expression* (QUITEL 2013)
   PLACE and YEAR: Granada (Spain), 2013

7. TYPE OF PRESENTATION: Poster
   AUTHORS: Javier Navarro-Ruiz, Albert Rimola, Mariona Sodupe
   TITLE: "H_2 formation on silicate surfaces of cosmic interest"
   CONGRESS: *3rd New trends in Computational Chemistry for Industry Applications*
   PLACE and YEAR: Barcelona (Spain), 2013

8. TYPE OF PRESENTATION: Poster
   AUTHORS: Javier Navarro-Ruiz, Albert Rimola, Mariona Sodupe
   TITLE: "Functionalization vs polymerization on H-terminated silicon surfaces. A B3LYP periodic Study"
   CONGRESS: *8th Congress on Electronic Structure: Principles and Applications* (ESPA2012)
   PLACE and YEAR: Barcelona (Spain), 2012

Supervision of Research Works

1. Master Thesis: "Computational study on the functionalization and polymerization processes on hydrogenated silicon surfaces". Javier Navarro Ruiz, Universitat Autònoma de Barcelona, 2012.

2. PhD Thesis: "Modelling of the interstellar dust and prebiotic molecule formation by means of ab inito simulations". Javier Navarro Ruiz, Universitat Autònoma de Barcelona, *in progress*.

3. Postdoctoral Work: "In silico prodection of the phsysico-chemical features of silicate cosmic dust". José Ángel Martínez-González, Universitat Autònoma de Barcelona.

Referee Activity

- Referee of manuscripts of international journals:

  Journal of Physical Chemistry (A, B, C and Letters), Physical Chemistry Chemical Physics, CrystEngComm, Journal of Molecular Modelling, Monthly Notices of the Royal Astronomical Society, Astronomy & Astrophysics, Molecular Physics, Journal of Physics and Chemistry of Solids.

- Evaluator of research projects:

  Agencia Nacional de Evaluación y Prospectiva (State Agency of Spain), Agencia Nacional de Promoción Científica y Tecnológica (State Agency of Argentina)

International Collaborations

- Nadia Balucani, University of Perugia
- Cecilia Ceccarelli, Observatory of Grenoble
- José Cernicharo, Institute
- Thierry Chiavassa, University Aix-Marseille
- Dominique Costa, École Nationale Supérieure de Chimie de Paris
- Roberto Dovesi, University of Turin
- Jean-Françoise Lambert, University Pierre et Marie Curie
- Zita Martins, Imperial College London
- Gianmario Martra, University of Turin
- Angelos Michaelides, University College London
- Valerio Pirronello, University of Catania
- Josep M. Trigo-Rodríguez, Institute of Space Sciences - CSIC
- Piero Ugliengo, University of Turin

Old Plan

Degree	Subject	Course	Kind of lecture	Total credits
Chemistry	Chemical Kinetics	2005/2006 2006/2007	Classroom problems	3.0
	Lab of Computational Chemistry	2004/2005 2005/2006 2006/2007	Laboratory	13.2
	Basics on Chemical Laboratory	2004/2005	Laboratory	2.1
	Laboratory of Thermodynamics	2006/2007	Laboratory	4.5
	Laboratory of Chemical Kinetics	2009/2010 2010/2011[a]	Laboratory	7.0
Environmental Sciences	Thermodynamics and Chemical Kinetics	2010/2011 2011/2012[a]	Classroom problems Theory	1.5 2.0
Biotechnology	Thermodynamics and Chemical Kinetics	2006/2007	Classroom problems	3.0
Vet	Chemistry	2006/2007	Laboratory	3.0

[a] Responsible of the subject

Current Plan (European Higher Education)

Degree	Subject	Course	Kind of lecture	Total ECTS
Chemistry	Spectroscopy	2011/2012[a] 2012/2013[a] 2013/2014[a]	Laboratory	4.85
	Analyisis and Determination of Properties	2013/2014	Laboratory	1.16
Nanoscience and Nanotech.	Bond chemistry and structure of matter	2010/2011 2011/2012	Classroom problems	3.54
	Molecular Spectroscopy	2012/2013[a] 2013/2014[a]	Theory	8.1
Genetics	Chemistry	2011/2012 2012/2013 2013/2014	Classroom problems	4.47

[a] Responsible of the subject

Science Dissemination Articles

1. Albert Rimola, Mariona Sodupe. "Síntesi de proteïnes en superficies de minerals per conèixer sobre l'origen de la vida". *Teraflop* 92, July **2007**, 8-10. (http://www.cesca.cat/sites/default/files/docs/tera93.pdf)

2. Cristina Rodríguez-Rodríguez, Albert Rimola, Jorge Alí-Torres, Pilar González-Duarte, Mariona Sodupe. "Estrategias in silico para el diseño y selección de compuestos con potencial aplicación en la enfermedad de Alzheimer". *Lifescienceslab*, Noviembre/Diciembre10, 66-68. (http://www.lifescienceslab.com/require/revistas-digitales/12/pdf/lifescienceslab-12.pdf)

3. Mariona Sodupe, Albert Rimola, Piero Ugliengo. "Adsorción y polimerización de aminoácidos en superficies de minerales. Simulaciones computacionales de procesos prebióticos". *Anales de Química*, **2011**, *107* (2), 137-143. (http://www.rseq.org/anales/numeros-atrasados/item/106-vol107-n%C2%BA-2-abril-junio-2011)

4. Albert Rimola. "Les simulacions al laboratori permeten entendre la composició dels cometes". *UAB Divulga*, **03/2015**. (https://intranet.uab.es/web?cid=1096481464166&pagename=UABDivulga%2FPage%2FTemplatePageDetallArticleInvestigar&param1=1345682685032)

Popular Science Speeches

Speeches in secondary schools within the framework of "**Talk and experience with someone who does research in Barcelona**", organized by *Observatory for the Science Dissemination of UAB*.

TITLE: "The Molecules of the Origin of Life"

SECONDARY SCHOOL: INS Eugeni d'Ors, Hospitalet de Llobregat (2011)
INS Menéndez y Pelayo, Barcelona (2012)
INS Margarida Xirgu, Hospitalet de Llobregat (2013)
INS Menéndez y Pelayo, Barcelona (2014)
INS Ferran Tallada, Barcelona (2014)

Participation in other Activities of Science Dissemination

- **Interactive Chemistry**: Hands-on lab sessions for students of secondary schools carried out in laboratories of the Dep. Chemistry of UAB.

My role focused on the planning and implementation of some hand-on experiences and leading the sessions (2011, 2012, 2013 and 2014).

- **Thanks to Chemistry**: Exposition organized by the Dep. Chemistry of UAB due to the International Year of Chemistry 2011.
  My role focused on the planning and building of some aspects of the exposition.

AWARDS AND OTHER MERITS

Awards

- **AWARD OF OUTSTANDING PhD THESIS**. Doctorate program of Theoretical and Computational Chemistry. Course 2006/07, UAB.

- **EUROPEAN DOCTORATE MENTION AWARD**

Accreditations from Teaching and Research Assessment Agencies

2008 Accreditation of **PROFESSOR LECTOR**
Granted by *Agència per a la Qualitat del Sistema Universitari de Catalunya* (AQU)

2011 Accreditation of **PROFESSOR AGREGAT**
Granted by *Agència per a la Qualitat del Sistema Universitari de Catalunya* (AQU)

Other Research Merits

- Responsible of an Application in the **ERC Starting Grant 2013** call. **Final score = A**, but not retained for funding.
  Title: In Silico prediction of the physico-chemical features of cosmic dust (DUSTAR, FP7 337052)

- **COVERS and BACK COVERS:**
  - *Physical Chemistry Chemical Physics*, **2009**, *11*, Issue 14
  - *Physical Chemistry Chemical Physics*, **2009**, *11*, Issue 40
  - *Physical Chemistry Chemical Physics*, **2010**, *12*, Issue 24
  - *Physical Chemistry Chemical Physics*, **2014**, *16*, Issue 8

- **HIGHLIGHTED ARTICLES:**
  Phys. Chem. Chem. Phys., **2009**, *11*, 2497 – 2506. **Highlighted** in *Chemical Science*, **2009**, *6*, C17.

- **INVITED PERSPECTIVE ARTICLE:**
  Phys. Chem. Chem. Phys., **2010**, *12*, 6309 – 6329.

- **COAUTHOR of an ONLINE TUTORIAL:**
  Title: Localization of Transition States with CRYSTAL09
  Authors: Albert Rimola, Claudio M. Zicovich-Wilson
  (http://www.crystal.unito.it/tutorials)

- **ORGANIZATION OF SCIENTIFIC CONFERENCES:**
  - XXVI Meeting of the Reference Network of Theoretical and Computational Chemistry. Bellaterra, 2010.

- WATOC Satellite “Theoretical Modeling of Materials”. Barcelona, 2011.

Other Teaching Merits

- Responsible for the design of the subject “**Molecular Spectroscopy**” belonging to the new degree of *Nanoscience and Nanotechnology* implemented in the European Higher Education plan. Course 2012/13, UAB.

- Reformulation of the classroom problems of the subject “**Thermodynamics and Chemical Kinetics**” of the degree of *Biotechnology*, within the innovation teaching project entitled “Treballem les competències en Química. Elaboració d’activitats i material docent per a una metodologia d’aprenentatge actiu a l’aula**”** headed by Dr. Jordi Gener. Course 2006/07, UAB.