

## Curriculum vitae

### PERSONAL INFORMATION Enrico Bodo

📍 Chemistry Department, University of Rome "La Sapienza". P. A. Moro 5, 00185 Rome, Italy

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📅 Date of birth 13 August 1972 | 🇮🇹 Nationality Italian

### ACADEMIC APPOINTMENTS

#### 2015—present Associate Professor

Associate Professor in Physical Chemistry at the University of Rome "La Sapienza" in the Chemistry Department.

#### 2004—2015 Assistant Professor

"Researcher" (a position equivalent to an American Assistant Professor) at the University of Rome "La Sapienza" in the Chemistry Department.

#### Invited Professor

2017 November Institut de Chimie Physique, CLIO, Université Paris Saclay, Orsay, France.

2015 June Institut de Chimie Physique, CLIO, Université Paris-Sud, Orsay, France.

#### Qualification

2016 Qualification for Full Professor in [Physical Chemistry](#).

2013 Qualification for Associate Professor in [Inorganic Chemistry](#) and in [Physical Chemistry](#).

#### Visits

2013—2014 Collaborator and recurring short-term visitor at [LAMBE](#) (Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement) Evry, Cedex, France.

2004—10 Collaborator and recurring short-term visitor at [ITAMP](#) (Harvard Smithsonian Center for Astrophysics) Cambridge Massachusetts, USA.

2001 Visiting fellow of the ITAMP institute under the supervision of Prof. A. Dalgarno, Harvard Smithsonian Center for Astrophysics, Cambridge, Massachusetts, USA.

### EDUCATION

#### 2002—2004 PostDoc

PostDoc in the theoretical chemistry group of Prof. Gianturco at the University of Rome "La Sapienza". Research project: [Dynamical studies of the energetic processes in molecular gases at ultra-low temperatures](#)

#### 1999—2001 PhD in Chemistry

University of Rome La Sapienza. Supervisor: Prof. F. A. Gianturco. Dissertation title: [The Lithium chemistry in the early Universe: quantum treatment of interactions and dynamics](#).

#### 1998 Master's Degree

*Laurea* (equivalent to an American Master's Degree) in Chemistry at the University of Rome "La Sapienza" achieved on the 21<sup>st</sup> May 1998 ([magna cum laude](#)).

**ACADEMIC COORDINATION AND ORGANIZATION**

- 2019—present Member of the "Research and Third mission" committee of the Chemistry Department  
2012—2020 Member of the committee for Assurance of Quality of the Faculty of Science.  
2011—present Member of the Permanent PhD committee of the Chemistry Department.

**TEACHING**

- 2017/18—present Course for the Degree in Chemistry at the University of Rome "La Sapienza": [Chemical Physics II](#) (9 credits).  
2010/11—present Course for the Degree in Chemistry at the University of Rome "La Sapienza": [Laboratory of Quantum Mechanics and Molecular Dynamics](#) (9 credits).  
2006/07—2009/10 Course for the Degree in Chemistry at the University of Rome "La Sapienza": [Quantum Mechanics](#) (50 hours).  
2006/07—2008/09 Course for the Degree in Chemistry at the University of Rome "La Sapienza": [Computer Science Technologies for Chemistry](#) (60 hours)  
2004/05—2009/10 Course for the Degree in Chemistry at the University of Rome "La Sapienza": [Application of Quantum Mechanics](#) (40 hours).

**SUPERVISOR ACTIVITIES****PhD Students and Postdoc**

- 2020—2023 PhD: Stefano Russo  
2020—2021 Postdoc: Andrea Le Donne  
2019—2022 PhD: Adriano Pierini, Mohammed Salha  
2018—2021 PhD: Henry Adenusi  
2017—2019 PhD: Andrea Le Donne  
2014-2015 Postdoc: Maria Montagna

**Master's Students**

- 2021 Federico Rottaro, Sara Marando, Gabriele Dilena, Vanessa Piacentini  
2020 Federica Angiolari, Alice Latini, Simone Amatori, Stefano Onofri  
2019 Adriano Pierini, Nicole Mancini, Martina Sebastianelli, Stefano Russo  
2005—2018 Aurora Ponzi, Gabriele Lanaro, Luigi Tiburzi, Mara Chiricotto, Silvana Vasile, Marco Pezzella, Veronica Macaluso, Flavio Siro Brigiano, Andrea Le Donne, Giulia Bovolenta

**EDITORIAL ACTIVITIES, MEMBERSHIP AND AWARDS**

- 2021—present Member of the Selection Panel in the STORIES Project (Storage Research Infrastructure Ecosystem) Horizon 2020.  
2020—present Member of the editorial board of [Molecules](#).  
2020—present Member of the editorial board of [Symmetry](#).  
2020 Guest Editor of the special issue [Theoretical Computational Description of Ionic Liquids](#) in *Molecules*.  
2020 Evaluator for the Executive Agency for Higher Education, Research, Development and Innovation Funding, (Bucarest, Romania). Programs: *Postdoctoral Research Projects (PD 2019)* and *Research Projects for Stimulating Young Independent Teams (TE 2019)*.  
2018 [Award](#) for Teaching Excellence from the Faculty of Science for the course of Physical Chemistry II (based on students opinions).  
2018 Referee for the German Research Foundation (DFG), (Bohn, Germany).  
2016 Evaluator for the Executive Agency for Higher Education, Research, Development and Innovation Funding, (Bucarest, Romania). Program *National Plan for Research, Development and Innovation for the period 2015 - 2020*.

- 2015 Referee for the [Materials Genome Initiative](#) of the US Department of Energy (Washington DC). Section "Computational Materials Sciences Program"
- 2012—present Referee for the Italian agency for research evaluation (ANVUR Italy).
- 2011—present Referee of the ISCRA, Italian SuperComputing Resource Allocation (CINECA, Bologna, Italy) .
- 2009—present EB is a referee for the following interanational journals: J. Phys. B, J Comp. Chem., Chem. Phys. Lett., Eur. J. Inorg. Chem., J. Chem. Phys., J. Phys. Chem., Phys. Chem. Chem. Phys., J. Mol. Struct., Surface Science, ChemPhysChem, Int. J. of Quant. Chem., Symmetry, ACS Omega, J. Comp. Chem. Organic and Biomolec. Chem., Electronic Structure, Appl. Materials and Interfaces, J. Mol. Liq., J. Phys. Cond. Matter., Symmetry, Molecules.
- 2009—present Member of the American Chemical Society.
- 2006—present Member of the Italian Society of Chemistry.

## FUNDING INFORMATION

### Research grants (received as the P.I.)

- 2018 Research Grant from "La Sapienza", University of Rome *Multidisciplinary study of intrinsic properties of model chiral molecules*: 55,000 €
- 2019 Visiting scientist grant from the University of Rome "Sapienza" for prof. G. Chass, QMUL, London, UK.
- 2017 Research Grant from "La Sapienza", University of Rome *Multidisciplinary study of intrinsic properties of chiral molecules*: 12,000 €
- 2015 Research Grant from "La Sapienza", University of Rome *Characterising new generation ionic liquids by theory and experiments: the role of phosphate and bi-sulphide groups on proton transfer and conductivity*: 30,000 €
- 2014 Research Grant from "La Sapienza", University of Rome *Aminoacid anions in organic compounds: exploring the boundary of room temperature ionic liquids*: 40,000 €
- 2011 Research Grant from "La Sapienza", University of Rome *The structure of metal-containing compounds in protic ionic liquids: theoretical and experimental studies*: 80,000 €
- 2008 Research grant from the Faculty of Science, "La Sapienza", University of Rome: *Elementary chemical reactions and molecular dynamics at low temperatures*: 4000 €
- 2009 Visiting scientist grant from the University of Rome "Sapienza" for prof. A. Belyaev, S. Peterburg Russia.
- 2007 Research grant from the Faculty of Science, "La Sapienza", University of Rome: *Elementary chemical reactions at ultra-low temperatures*: 4000 €
- 2007 Research Grant from CASPUR: 12 month post-doc position bursary employed by S. Orlandini: 12000 €

### Computational grants (received as the P.I.)

- 2017 [PRACE](#) (Partnership for advanced computing in Europe) Tier-0 Grant of 30,000,000 corehours. Project title: *Exploring Proton Transfer in Ionic Liquids*
- 2014 [PRACE](#) (Partnership for advanced computing in Europe) Tier-0 Grant of 27,000,000 corehours. Project title: *Amino-acid anions in organic compounds: charting the boundary of room temperature ionic liquids*
- 2013 [PRACE](#) (Partnership for advanced computing in Europe) Tier-0 Grant of 18,000,000 corehours. Project title: *Ab initio molecular dynamics of lanthanides in protic ionic liquids*.
- 2007-2018 many different computational projects from CASPUR (Rome) and from Cineca (Bologna) for a total of about 4,000,000 corehours on various architectures.

## SUMMARY OF SCIENTIFIC ACHIEVEMENTS

E. B. is coauthor of [127 publications](#) on international refereed journals and [5 book chapters](#). His *h-index* is [27](#) (Scopus) and has collected a total of around [2300 citations](#) (Scopus).

SELECTED PUBLICATIONS  
(ONLY RECENT)

- 2020 S. Onofri, A. Le Donne, H. Adenusi, E. Bodo\* *CO<sub>2</sub> Capture in Ionic Liquids Based on Amino Acid Anions With Protic Side Chains: a Computational Assessment of Kinetically Efficient Reaction Mechanisms*, *ChemistryOpen*, **9**, 1153 – 1160 (2020)
- A. Pierini, S. Brutti and E. Bodo\* *Superoxide Anion Disproportionation Induced by Li<sup>+</sup> and H<sup>+</sup>: Pathways to <sup>1</sup>O<sub>2</sub> Release in Li-O<sub>2</sub> Batteries*, *ChemPhysChem*, **21**, 2060 – 2067 (2020).
- H. Adenusi, G. Chass and E. Bodo\* *Theoretical Insights into the Structure of the Aminotris-(Methylenephosphonic Acid) (ATMP) Anion: A Possible Partner for Conducting Ionic Media*, *Symmetry*, **12**, 920 (2020)
- H. Adenusi, A. Le Donne, F. Porcelli and E. Bodo\* *Ab Initio Molecular Dynamics Study of Phospho-Amino Acid-Based Ionic Liquids: Formation of Zwitterionic Anions in the Presence of Acidic Side Chains*, *J. Chem. Phys. B.*, **124**, 1955-1964, (2020)
- E. Bodo\*, *Structural Features of Triethylammonium Acetate through Molecular Dynamics*, *Molecules*, **25**, 1432 (2020)
- 2019 E. Bodo, G. Bovolenta, C. Simha, R. Spezia *On the formation of propylene oxide from propylene in space: gas-phase reactions*, *Theor. Chem. Acc.*, **138**, 97 (2019)
- A. Le Donne, H. Adenusi, F. Porcelli and E. Bodo\* *Structural Features of Cholinium Based Protic Ionic Liquids through Molecular Dynamics*, *J. Phys. Chem. B*, **123**, 5568-5576 (2019).
- 2018 A. Le Donne, H. Adenusi, F. Porcelli, and E. Bodo\*, *Hydrogen Bonding as a Clustering Agent in Protic Ionic Liquids: Like-Charge vs Opposite-Charge Dimer Formation*, *ACS Omega* **3**, 10589-10600, (2018)
- M. Competella, A. Le Donne, M. Daniele, L. Gontrani, S. Lupi, E. Bodo\* and F. Leonelli, *Hydrogen Bonding Features in Cholinium-Based Protic Ionic Liquids from Molecular Dynamics Simulations*, *J. Phys. Chem. B*, **122**, 2635-2645, (2018).
- E. Bodo\*, A. Le Donne *Isomerization patterns and proton transfer in ionic liquids constituents as probed by ab-initio computation*, *J. Mol. Liq.*, **249**, 1075-1082 (2018)
- 2017 M. Montagna, R. Spezia, E. Bodo\* *Solvation Properties of the Actinide Ion Th(IV) in DMSO and DMSO:Water Mixtures through Polarizable Molecular Dynamics*, *Inorg. Chem.* **56**, 11929-11937 (2017)
- M. Montagna, R. Spezia and E. Bodo\*, *Structural and energetic properties of La<sup>3+</sup> in water/DMSO mixtures*, *J. Mol. Struct.* **1148**, 381-387, (2017)
- M. Competella, M. Montagna, L. Gontrani, E. Scarpellini and E. Bodo\*, *Unexpected Proton Mobility in the bulk phase of Cholinium-based Ionic Liquids. New Insights from Theoretical Calculations*, *Phys. Chem. Chem. Phys.* **19**, 11869 - 11880, (2017)
- 2016 D. Scuderi, E. Bodo, B. Chiavarino, S. Fornarini, M. E. Crestoni *Amino-acids oxidation: a combined study of cysteine oxo-forms by IRMPD spectroscopy and simulations*, *Chem. Eur. J.* **22**, (2016)
- 2015 E. Bodo\*, R. Spezia and V. Macaluso, *Solvent Structure Around Lanthanoids(III) Ions in Liquid DMSO as Revealed by Polarizable Molecular Dynamics Simulations*, *J. Phys. Chem. B.*, **119**, 13347-13357 (2015)
- E. Bodo\*, *Lanthanum(III) and Lutetium(III) in Nitrate-based Ionic Liquids: A Theoretical Study of Their Coordination Shell* *J. Phys. Chem. B.*, **119**, 11833-11838 (2015)
- 2014 E. Bodo, A. Ciavardini, A. Dalla Cort, I. Giannicchi, F. Yafteh Mihan, S. Fornarini, S. Vasile, D. Scuderi, S. Piccirillo, *Anion recognition by uranyl-salophen derivatives as probed by IRMPD spectroscopy and ab-initio modeling*. *Chem. Eur. J.*, **20**, 11783 - 11792, (2014).
- A. Benedetto, E. Bodo\*, L. Gontrani, P. Ballone and R. Caminiti, *Amino-acid anions in organic ionic compounds. An ab-initio study of selected ion pairs*, *J. Phys. Chem. B*, **118**, 2471, (2014).

## THIRD MISSION

- 2019—present Member of the "Research and Third mission" committee of the Chemistry Department
- 11-Nov-2019 Speaker at the *Giornata per i 150 anni della Tavola Periodica degli Elementi*, Area della Ricerca di Roma 1, CNR, Montelibretti. This was an educational event for high school students.

- 2-Dec-2019 Speaker at the "Christmas Seminars" held at the Chemistry Department of "La Sapienza", Rome. This was an educational event for high school students.

#### ORGANIZED NATIONAL AND INTERNATIONAL CONFERENCES

- 2019 XLVII Congresso Nazionale della Divisione di Chimica Fisica, La Sapienza, Rome, (July 1-3, 2019).
- 2015 III Convegno Divisione Chimica Teorica e Computazionale, CNR, Rome (December 14-16, 2015).
- 2008 Control Of Molecular Processes Induced by Electrons and Photons: Experiments and Interpretations A Congress in honor of Prof. Hotop, Beniamino Segre Interdisciplinar Center Accademia Nazionale dei Lincei, Rome, (October 2-4, 2008).
- 2005 EPIC-EIPAM 2005 Meeting, Joint conference for the EPIC and EIPAM EU networks, S. Martino al Cimino, Italy (June 25-30 2005).
- 2003 Theoretical concepts and recent experimental results on cold molecules, Volterra, Italy, (September 22-27, 2003).

#### LECTURES AND SEMINARS (ONLY RECENT)

- 2020 Oral presentation: *Isomerization patterns and proton transfer in ionic liquids: toward new conducting media*, Workshop of the division of Physical Chemistry of the Italian Chemical Society (14-15 December 2020)
- Invited Seminar: *Isomerization patterns and proton transfer in ionic liquids: crossing the boundary between the ionic and neutral phase*. Helmholtz Institute Ulm (HIU) Electrochemical Energy Storage Ulm, Germany. (November 3, 2020)
- 2018 Oral presentation: *Isomerization patterns and proton transfer in the molecular constituents of protic ionic liquids probed by ab-initio computations*. 6th International Conference on Ionic Liquids for Electrochemistry, Rome, Italy (ILED-6) (September 9-11, 2018).
- Invited lecture: *New insights in protic ionic liquids from theoretical calculations*. International Workshop on Soft Matter and Biophysics Theories, Beijing, China (January 28-31, 2018).
- 2017 Oral presentation: *Proton Mobility in Protic Ionic Liquids: New Results from Theoretical Calculations* XXIX IUPAP Conference in Computational Physics (CCP2017), University Pierre et Marie Curie - Sorbonne, Paris, France (July 9-13, 2017)
- 2017 Oral presentation: *Proton mobility in protic Ionic Liquids*. III Congresso della Divisione di Chimica Teorica e Computazionale, Pisa, Italy (October 2-5, 2016).
- 2016 Oral presentation: *The structure of ionic liquids from molecular dynamics: recent results*. International Meeting on Ionic Liquids for Electrochemical Devices ILED, Rome, Italy (July 11-13 2016).
- 2015 Invited lecture: *The Structure of Ionic Liquids from Molecular Dynamics: Recent Results*. XVIII – Simposio Brasileiro de Quimica Teorica, Pirenopolis, Goias, Brasil (November 22-25 2015).
- Oral presentation: *Ionic liquids from a molecular perspective*. CMAST Workshop: Computational Materials Science and Technology. CRESCOENEA, Italy, (April 13, 2015).
- 2014 Oral presentation: *Amino Acid Anions in Organic Ionic Compounds: Charting the Boundary of Room Temperature Ionic Liquids*. Winter Modeling, Modena, Italy (March 13-14, 2014).
- 2013 Oral presentation: *Ionic liquids from a molecular perspective*. XLI Congresso della Divisione di Chimica Fisica, Alessandria, Italy. (June 25-27, 2013).
- Oral presentation: *Ionic liquids from a molecular perspective*. II Congresso della Divisione di Chimica Teorica e Computazionale, Padova, Italy (February 20-22, 2013).
- 2012 Invited Seminar: *The Structure of Ionic Liquids from a Molecular Perspective*. The Analysis and Modeling laboratory for Biology and Environment (LAMBE), Univ. of Évry-val-d'Essonne, Evry Cedex, France, (November 2012).
- 2011 Oral presentation: *The structure of ionic liquids based on geminal imidazolium: a theoretical study*. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce, Italy (September 11-16, 2011).

Oral presentation: *Theoretical simulations of ionic liquids*. 110th Bunsentagung (Annual German Conference on Physical Chemistry), invitation in the special EuChemMS session, Freien Universität Berlin, Germany (June 2-4, 2011)

- 2010 Oral presentation: *Atomistic Simulation of Ionic Liquids: Dissecting Their Local Structure with Combined Experimental and Theoretical Determinations*. XXXIX Congresso Nazionale della Divisione di Chimica Fisica, Stresa, Italy (September 20-24, 2010).

Oral presentation: Atomistic simulations of imidazolium-based ionic liquids: current challenges for theoretical models. International conference on Ionic Liquids for Electrochemical Devices (ILED-2), CNR, Roma, Italy (2010).

Oral presentation: *The stereochemistry of sulphoxides: theoretical treatment of the inversion process*. 8th workshop on Molecular Theories and simulations, Gaeta, Italy (May 24-26 2010).