Curriculum vitae

PERSONAL INFORMATION

Enrico Bodo

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ORCID 0000-0001-8449-4711

Date of birth 13 August 1972 | Nationality Italian

PERSONAL SKILLS

Mother tongue	Italian
Other languages	English, fluent

DIGITAL SKILLS

Operating systems	Unix/Linux (advanced), MacOsX, Windows
Programming	Fortran (advanced), Bash scripting

ACADEMIC APPOINTMENTS

Dec 2023—today	Full Professor in Physical Chemistry at the University of Rome La Sapienza in the Chemistry Department.
2015—2023	Associate Professor in Physical Chemistry at the University of Rome La Sapienza in the Chemistry Department.
2004—2015	"Researcher" (Assistant Professor) at the University of Rome La Sapienza in the Chemistry Department.
2002 April—2003 December	PostDoc in the theoretical chemistry group of Prof. Gianturco at the University of Rome La Sapienza in the Chemistry Department. Research project: Dynamical studies of the energetic processes in molecular gases at ultra-low temperatures

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 and 2023	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

1999—2001	PhD in Chemistry, Department of 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.

21-May-1998 *Laurea* (equivalent to a Master's Degree) in Chemistry at the University of Rome La Sapienza (magna cum laude).

ACADEMIC COORDINATION AND ORGANIZATION

12/2022—present Elected member of the Board of the Theoretical and Computational Chemistry Division of the Italian Chemical Society

12/2020—12/2022 Elected member of the Board of the Faculty of Science of the University of Rome La Sapienza

2019—present Member of the Research and outreach committee of the Chemistry Department of the University of Rome La Sapienza

2012—2020 Member of the committee for Quality Assurance of the Faculty of Science of the University of Rome La Sapienza

2011—present Member of the graduate studies (PhD) committee of the Chemistry Department of the University of Rome La Sapienza

TEACHING ACTIVITIES

2021/22—present Course for the Bachelor Degree in Chemical Sciences at the University of Rome La Sapienza: Chemical Physics II (9 credits).

2020 Teaching excellence award conferred by the Faculty of Sciences for the course of Physical Chemistry II. The award is based on the results of the student questionnaires.

2018 Teaching excellence award conferred by the Faculty of Sciences for the course of Physical Chemistry II. The award is based on the results of the OPIS questionnaires.

2017/18—2020/2021 Course for the Bachelor Degree in Chemistry at the University of Rome La Sapienza: Chemical Physics II (9 credits).

AA 2015/16—–2016/17 Course for the Bachelor Degree in Chemistry at the University of Rome La Sapienza: Chemical Physics III (3 credits).

2015 Course for the Chemical Science PhD school: "*Density Functional Theory: a guide for the study of complex materials*" (3 credits).

2010/11—present Course for the Master's Degree in Chemistry at the University of Rome La Sapienza: Laboratory of Quantum Mechanics and Molecular Dynamics (9 credits).

2006/07—2008/09 Course for the Master's Degree in Chemistry at the University of Rome La Sapienza: Quantum Mechanics (50 hours).

2006/07—2008/09 Course for the Master's Degree in Chemistry at the University of Rome La Sapienza: Computer Science Technologies for Chemistry (50 hours).

2004/05—2009/10 Course for the Master's Degree in Chemistry at the University of Rome La Sapienza: Application of Quantum Mechanics (40 hours).

Outreach and Third Mission Activities

19-Set-2023 Speaker for the *Research Nights* with a lecture entitled The origin of the periodic table elements, Department of Chemistry of La Sapienza. This was an educational event for high school students.

21-Dic-2022 Speaker at the *Christmas Seminars* held at the Chemistry Department of La Sapienza, with a lecture entitled The voyage of a proton in the universe. This was an educational event for high school students.

19-Set-2022 Speaker for the *Research Nights* with a lecture entitled The elements of the periodic table, Department of Mathematics of La Sapienza. This was an educational event for high school students.

5-May-2022 Invited speaker to the *Space, last frontier*, a series of conferences, organized by Discovery Link, with a lecture on astrochemistry held at the Chemistry Department of La Sapienza

30-Nov-2021 Speaker at *Lezioni a Palazzo* for the project "Tre Stazioni per Arte-Scienza", Palaexpo, Rome. Educational event held inside the Palaexpo museum for a general public.

11-Nov-2019 Speaker at the *Giornata per i 150 anni della Tavola Periodica degli Elementi*, Rome 1 Research Area, 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, with a lecture entitled The history of the atoms from the Big Bang to today. This was an educational event for high school students.

PhD Students and Postdoc

2023—2026 PhD: Alessandro Azzali

PhD: Francesca D'Ambrosio

2023—2025 Postdoc: Adriano Pierini

2022–2025 PhD: Matteo Farina (Prof. I. Daidone, co-supervisor)

PhD: Marcello Della Sala (Prof. P. D'Angelo, co-supervisor)

2021—2024 PhD: Vanessa Piacentini

2020—2023 PhD: Stefano Russo, Polarizable Force Field for amino acid based ionic liquids: An extension of AMOEBA force field

2020—2021 Postdoc: Andrea Le Donne

2019—2022 PhD: Adriano Pierini, Computational study of electron-transfers and singlet oxygen in aprotic metal-O2 batteries.

PhD: Mohammed Salha, (Prof. G. Chass, co-supervisor), Constitution, Configuration and Conformation: Molecular engineering of tougher cement.

2018—2021 PhD: Henry Adenusi, Proton Transfer Mechanisms in Protic Ionic Liquids.

2017—2019 PhD: Andrea Le Donne, Study of Dry Proton Mobility Inside Liquids: the Particular Case of Amino Acid-Based Ionic Liquids.

2014-2015 Postdoc: Maria Montagna

Master's Students

2024 Eleonora Zucca

2023 Alessandro Azzali, Aurora Capitani, Francesca D'Ambrosio

2022 Leonardo Biancorosso, Simone Pistillo, Guido Giannetti

2021 Sara Marando, Gabriele Dilena, Vanessa Piacentini, Matteo Farina

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

EVALUATIONS ACTIVITIES AND MEMBERSHIPS

2023 Evaluator for the Executive Agency for Higher Education, Research, Development and Innovation Funding (UEFISCDI), Bucarest, Romania. Program: *PNRR-I8-2022*.

2022 Evaluator for the National Science Centre Poland, Poland, Program: *OPUS-23*, Panel ST8.

2021–present Evaluator for the Executive Agency for Higher Education, Research, Development and Innovation Funding (UEFISCDI) Bucarest, Romania. Programs: *Postdoctoral Research Projects (PD 2021) and Research Projects for Stimulating Young Independent Teams (TE 2021)*.

2021—present Member of the Selection Panel in the STORIES Project (Storage Research Infrastructure Ecosystem) Horizon 2020.

2020 Evaluator for the Executive Agency for Higher Education, Research, Development and Innovation Funding (UEFISCDI), Bucarest, Romania. Programs: *Postdoctoral Research Projects (PD 2019) and Research Projects for Stimulating Young Independent Teams (TE 2019)*.

2018 Referee for the German Research Foundation (DFG), (Bohn, Germany).

2016 Evaluator for the Executive Agency for Higher Education, Research, Development and Innovation Funding (UEFISCDI), 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 many international journals, such as: 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—2019 Member of the American Chemical Society.

2006—present Member of the Italian Society of Chemistry.

EDITORIAL ACTIVITIES

2022 *Guest Editor* of the special issue Ionic Liquids and Deep Eutectic Solvents: Greener Approaches for Sustainable Chemistry in *Symmetry*.

Nov. 2021—oggi *Editor in chief* of Liquids.

2020—oggi Membro del comitato editoriale di Molecules (WOS IF 4.927, indicizzata Scopus).

2020—oggi Membro del comitato editoriale di Symmetry (WOS IF 2.940, indicizzata Scopus).

2020 Guest Editor of the special issue Theoretical Computational Description of Ionic Liquids in *Molecules*.

FUNDING INFORMATION

Research grants (received as the P.I.)

2023 Financial support of 50000 Euro for a PhD bursary from "CloudWise" company for the *Development of Machine Learning force fields for the characterization and the design of electrolytes for new generation solid-state batteries.*

2018 Research Grant fromLa Sapienza, University of Rome *Exploring Proton Transfer in Biocompatible Protic Ionic Liquids with Computational Methods*: 15000 Euro.

2018 Research Grant from La Sapienza, University of Rome *Multidisciplinary study of intrinsic properties of model chiral molecules*: 54,000 €

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*: 51,000 €

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 €

Computational grants (received as the P.I. with peer-review)

2022 HPC-access: Tier-0 grant of 6.400.000 corehours. *Polarizable Molecular Dynamics of Biocompatible Ionic Liquids.*

2021 PRACE (Partnership for advanced computing in Europe) Tier-0 Grant of 3,200,000 corehours. Project title: *Understanding the Role of Aluminium in Cements by Ab-initio Modelling*

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—today many different computational projects from CASPUR (Rome) and from Cineca (Bologna) for a total of about 4,000,000 core/hours on various architectures.

Participation to other grants

2022— National center 4, spoke 13, project: *Enabling technologies for sustainable mobility: electrochemical energy storage and electric traction*

2022— Extended network 2, spoke 9, project: *Energy-Sustainable Advanced Materials: from theoretical design to experimental synthesis and characterization*

2021 European project SIGNE, Composite Silicon/Graphite Anodes with Ni-Rich Cathodes and Safe Ether based Electrolytes for High Capacity Li-ion Batteries Horizon Europe Framework Programme

2017 National project PRIN 2017: *Cutting-edge X-ray methods and models for the understanding of surface site reactivity in heterogeneous catalysts and sensors*

2009 National project PRIN 2009: *Structural characterization of ionic liquids between -200 and 200 Celsius degrees temperatures*

2006 National project PRIN 2006: *Theoretical models and computational methods for the study of molecular processes at low and ultra-low temperature*

2006 National project ecvhighlightPRIN 2004: *Theoretical models and computational methods of the quantum structures and dynamics in molecules and molecular aggregates in neutral and ionized forms*

SUMMARY OF SCIENTIFIC ACHIEVEMENTS

E. B. is coauthor of 150 publications on international refereed journals and 5 book chapters. His h-index is 30 (source Scopus) and has collected a total of around 2865 citations (source Scopus).

ORGANIZATION AND CHAIRS AT NATIONAL AND INTERNATIONAL CONFERENCES

2023 Scientific Commitee for the VIII National Congress of Theoretical and Computational Chemistry Division, Pisa (September 20-22).

2022 Conference Chair of the First Symposium for YouNg Chemists: Innovation and Sustainability (SYNC2022), Chemistry Department, La Sapienza, Rome (June, 20-23).

2019 Organizing committee: XLVII National Congress of the Physical Chemistry Division of the Italian Chemical Society, La Sapienza, Rome, (July 1-3).

2015 Organizing committee of the III Congress of the Division of Theoretical and Computational Chemistry of the Italian Chemical Society, CNR, sede centrale, Rome (December 14-16).

2008 Organizing committee: 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).

2005 Organizing committee: EPIC-EIPAM 2005 Meeting, Joint conference for the EPIC and EIPAM EU networks, S. Martino al Cimino, Italy (June 25-30).

2003 Organizing committee: Theoretical concepts and recent experimental results on cold molecules, Volterra, Italy, (September 22-27).

LECTURES AND SEMINARS (ONLY RECENT)

2023 Keynote Speaker: *Computational modeling of new generation batteries: a study of parasitic chemistries and of electrolytes properties.*, XLIX National Congress of Physical Chemistry Physical Chemistry: a fresh glimpse into the microscopic world, Torino (4-7 September 2023).

2023 Invited Lecture: *Investigating gas-phase reactive pathways toward polyatomic molecules in the interstellar medium*, Winter Modeling 2023 - New frontiers in astrochemistry and astrobiology, Naples (February 22-23, 2023)

2022 Invited lecture: *Computational approaches for biocompatible ionic liquids.*, VII Congress of the Division of Theoretical and Computational Chemistry of the Italian Chemical Society, Modena (September, 21-24, 2022)

2022 Invited lecture: *Computational studies of the reactive pathways leading to the parasitic release of singlet oxygen in metal-air batteries*, XLVIII National Conference of the Physical Chemistry Division of the Italian Chemistry Society., Genova (4-7 July 2022)

2022 Oral presentation: *Biocompatible and green ionic liquids: a computational description, challenges and perspectives*, XIII Convegno INSTM sulla Scienza e Tecnologia dei Materiali, Sestriere (TO) (23 al 26 January 2022)

2021 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, 2021)

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)

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, Bejing, 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 Quımica 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 Societá 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).

PUBLICATION LIST

151. A. Petrongari, V. Piacentini, A. Pierini, P. Fattibene, C. De Angelis, E. Bodo, and S. Brutti, *Insights into the LiI Redox Mediation in Aprotic Li–O2 Batteries: Solvation Effects and Singlet Oxygen Evolution*, ACS Appl. Mater. Interfaces, (2023)
https://doi.org/10.1021/acsami.3c12330

150. A. Pierini, A. Petrongari, V. Piacentini, S. Brutti, E. Bodo* *A Computational Study on Halogen/Halide Redox Mediators and Their Role in $^1O_2$ Release in Aprotic Li–O_2 Batteries*, J. Phys. Chem. A, **127**, 9229–9235, (2023)
https://doi.org/10.1021/acs.jpca.3c05246

149. M. Salha, H. Adenusi, J. H. Dupuis, E. Bodo, B. Botta, I. McKenzie, R. Y. Yada, D. H. Farrar, J. Magolan, K. V. Tian, G. A. Chass, *Bioactivity of the cannabigerol cannabinoid and its analogues – the role of 3-dimensional conformation*, Org. Biomol. Chem., **21**, 4683-4693, (2023)
https://doi.org/10.1039/D3OB00383C

148. G. Dilena, S. Pistillo and E. Bodo*, *About the Formation of NH_2OH^+ from Gas Phase Reactions under Astrochemical Conditions*, Molecules, **28**, 2932, (2023)
https://doi.org/10.3390/molecules28072932

147. M. S. Salha, R. Y. Yada, D. H. Farrar, G. A. Chass, K. V. Tian and E. Bodo, *Aluminium catalysed oligomerisation in cement-forming silicate systems*, Phys. Chem. Chem. Phys., **25**, 455-461 (2023)
https://doi.org/10.1039/d2cp03918d

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146. Y. Jiang, S. Indrajith, A. F. P. Mellor, T. Bürgi, M. Lecouvey, C. Clavaguéra, E. Bodo, C. Houée-Levin, E. Loire, G. Berden, J. Oomens, and D. Scuderi, *Final Products of One-Electron Oxidation of Cyclic Dipeptides Containing Methionine Investigated by IRMPD Spectroscopy: Does the Free Radical Choose the Final Compound?*, J. Phys. Chem. B, **126**, 10055–10068 (2022)
https://doi.org/10.1021/acs.jpcb.2c06541

145. A. Di Sabato, F. D'Acunzo, D. Filippini, F. Vetica, A. Brasiello, D. Corinti, E. Bodo, C. Michenzi, E. Panzetta, and P. Gentili, *Unusually Chemoselective Photocyclization of 2-(Hydroxyimino)aldehydes to Cyclobutanol Oximes: Synthetic, Stereochemical, and Mechanistic Aspects*, J. Org. Chem. (2022), **87**, 13803–13818
https://doi.org/10.1021/acs.joc.2c01503

144. M. Fuse, G. Longhi, G. Mazzeo, S. Stranges, F. Leonelli, G. Aquila, E. Bodo, B. Brunetti, C. Bicchi, C. Cagliero, J. Bloino, and S. Abbate *Anharmonic Aspects in Vibrational Circular Dichroism Spectra from 900 to 9000 cm^{-1} for Methyloxirane and Methylthiirane*, J. Phys. Chem. A, **126**, 6719–6733, (2022)
https://doi.org/10.1021/acs.jpca.2c05332

143. S. Russo, E. Bodo*, *A polarisable force field for bio-compatible ionic liquids based on amino acids anions* , Mol. Simul., **48**, 1650-1659 (2022)
https://doi.org/10.1080/08927022.2022.2113810

142. V. Piacentini, A. Le Donne, S. Russo and E. Bodo*, *A Computational Analysis of the Reaction of SO2 with Amino Acid Anions: Implications for Its Chemisorption in Biobased Ionic Liquids* Molecules, **27**, 3604, (2022)
https://doi.org/10.3390/molecules27113604

141. P. O'Keeffe, D. Catone, S. Turchini, A. Paladini, A.Dalla Cort, E. Bodo and S. Piccirillo, *Excited state dynamics of Zn–salophen complexes*, Photochem. Photobiol. Sci., **21**, 923–934, (2022)
https://doi.org/10.1007/s43630-021-00165-0

140. E. Bodo*, *Perspectives in the Computational Modeling of New Generation, Biocompatible Ionic Liquids*, J. Phys. Chem. B, **126**, 3–13 (2022)
https://doi.org/10.1021/acs.jpcb.1c09476

139. A. Le Donne, S. Russo, E. Bodo*, *Assessing the Propensity Toward Ionization in Nanosized Clusters of Protic Ionic Liquids by Ab-initio Methods*, Chem. Phys., **552**, 111365 (2022)
https://doi.org/10.1016/j.chemphys.2021.111365

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138. (Editorial) E. Bodo *Welcome to Liquids: An Open Access Journal*, Liquids , **1**, 75-76 (2021)

137. A. Pierini, S. Brutti, and E. Bodo*, *Reactions in non-aqueous alkali and alkaline-earth metal-oxygen batteries: a thermodynamic study*, Phys. Chem. Chem. Phys., **23**, 24487 - 24496 (2021)
https://doi.org/10.1039/D1CP03188K

136. A. Pierini, S. Brutti, and E. Bodo*, *Study of the Electronic Structure of Alkali Peroxides and Their Role in the Chemistry of Metal–Oxygen Batteries*, J.Phys. Chem. A, **125**, 9368–9376 (2021)
https://doi.org/10.1021/acs.jpca.1c07255

135. A. Pierini, S. Brutti and E. Bodo*, *Reactive pathways toward parasitic release of singlet oxygen in metal-air batteries*, npj Computational Materials **7**, 126 (2021)
https://doi.org/10.1038/s41524-021-00597-3

134. F. Ripanti, C. Fasolato, F. Mazzarda, S. Palleschi, M. Ceccarini, C. Li, M. Bignami, E. Bodo, S. E. J. Bell, F. Mazzei, and P. Postorino, *Advanced Raman Spectroscopy Detection of Oxidative Damage in Nucleic Acid Bases: Probing Chemical Changes and Intermolecular Interactions in Guanosine at Ultralow Concentration*, Anal. Chem., **93**, 10825-10833, (2021).
https://doi.org/10.1021/acs.analchem.1c01049

133. S. Onofri and E. Bodo* *CO_2 Capture in Biocompatible Amino Acid Ionic Liquids: Exploring the Reaction Mechanisms for Bimolecular Absorption Processes*, J. Phys. Chem. B, **125**, 5611–5619, (2021).
https://doi.org/10.1021/acs.jpcb.1c02945

132. A. Le Donne, H. Adenusi, F. Porcelli and E. Bodo*, *Hydrogen bonding in biocompatible ionic liquids: an ab-initio characterization of dimeric interactions*, Electronic Structure, **3**, 025004, (2021).
https://doi.org/10.1088/2516-1075/abfd21

131. E. Bodo*, *Modelling biocompatible ionic liquids based on organic acids, and amino acids: challenges for computational models and future perspectives*, Org. Biomol. Chem., **19**, 4002-4013, (2021).
https://doi.org/10.1039/D1OB00011J

130. A. Le Donne, E. Bodo*, *Cholinium amino acid-based ionic liquids*, Biophys Rev, **13**, 147-160, (2021).
https://doi.org/10.1007/s12551-021-00782-0

129. E. Bodo*, M. Bonomo, and A. Mariani, *Assessing the Structure of Protic Ionic Liquids Based on Triethylammonium and Organic Acid Anions*, J. Phys. Chem. B, 125, 2781–2792, (2021)
https://doi.org/10.1021/acs.jpcb.1c00249

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128. S. Onofri, A. Le Donne, H. Adenusi, E. Bodo* *CO_2 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).
https://doi.org/10.1002/open.202000275

127. A. Pierini, S. Brutti and E. Bodo* *Superoxide Anion Disproportionation Induced by Li^+ and H^+: Pathways to $^1O_2$ Release in Li-O_2 Batteries*, ChemPhysChem, **21**, 2060 – 2067 (2020).
https://doi.org/10.1002/cphc.202000318

126. 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).
https://doi.org/10.3390/SYM12060920

125. 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).
https://doi.org/10.1021/acs.jpcb.9b09703

124. E. Bodo*, *Structural Features of Triethylammonium Acetate through Molecular Dynamics*, Molecules, **25**, 1432 (2020).
https://doi.org/10.3390/molecules25061432

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123. 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).
https://doi.org/10.1007/s00214-019-2485-3

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