Curriculum vitae

PERSONAL INFORMATION

Enrico Bodo

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

enrico.bodo@uniroma1.it

https://sites.google.com/uniroma1.it/enricobodo/home

ORCID 0000-0001-8449-4711

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 21st May 1998 (magna cum laude).

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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).

THIRD MISSION

30-Nov-2021 Speaker at "Lezioni a Palazzo" for the project "Tre Stazioni per Arte-Scienza", Palaexpo, Roma .

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*, Research area of Rome 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.

SUPERVISOR ACTIVITIES

PhD Students and Postdoc

2021—2024 PhD: Vanessa Piacentini

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

2022 Leonardo Biancorosso

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

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 AND EVALUATIONS ACTIVITIES, MEMBERSHIPS AND AWARDS

Nov. 2021—present Chief editor and Founding editor of Liquids.

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2021 Evaluator for the Executive Agency for Higher Education, Research, Development and Innovation Funding, (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 Award for Teaching Excellence from the Faculty of Science for the course of Physical Chemistry II (based on students opinions).

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 international 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*: 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 €

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2007 Research Grant from CASPUR: 12 month post-doc position bursary employed by S. Orlandini: 12000 €

Computational grants (received as the P.I.)

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.*

2007-2018 many different computational projects from CASPUR (Rome) and from Cineca (Bologna) for a total of about 4,000,000 corehours on various architectures.

Participation to other grants

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*

SUMMARY OF SCIENTIFIC ACHIEVEMENTS

E. B. is coauthor of 140 publications on international refereed journals and 5 book chapters. His h-index is 29 (source Scopus) and has collected a total of around 2540 citations (source Scopus).

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)

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)

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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)

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, 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).

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PUBLICATION LIST

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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122. 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). https://doi.org/10.1021/acs.jpcb.9b03314

121. A. Ciavardini, M. Coreno, C. Callegari, C. Spezzani, G. De Ninno, B. Ressel, C. Grazioli, M. de Simone, A. Kivimaki, P. Miotti, F. Frassetto, L. Poletto, C. Puglia, S. Fornarini, E. Bodo , M. Pezzella and S. Piccirillo, *Ultra-Fast-VUV Photoemission Study of UV Excited 2-Nitrophenol*, J. Phys. Chem. A, **123**, 1295-1302 (2019). https://doi.org/10.1021/acs.jpca.8b10136

120. D. Corinti, A. Maccelli, B. Chiavarino, P. Maitre, D. Scuderi, E. Bodo, S. Fornarini, and Maria Elisa Crestoni *Vibrational signatures of curcumin's chelation in copper(II) complexes: An appraisal by IRMPD spectroscopy* J. Chem. Phys. **150**, 165101 (2019). https://doi.org/10.1063/1.5086666

119. B. D. Linford, A. Le Donne , D. Scuderi, E. Bodo and Travis D Fridgen, *Strong intramolecular hydrogen bonding in protonated b-methylaminoalanine: A vibrational spectroscopic and computational study*, Eur. J. Mass Spectr., **25**, 133-141, (2019). https://doi.org/10.1177/1469066718791998

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118. 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). https://doi.org/10.1021/acsomega.8b01615

117. M. C. Castrovilli, P. Bolognesi, E. Bodo, G. Mattioli, A. Cartonib and L. Avaldi *An experimental and theoretical investigation of XPS and NEXAFS of 5-halouracils*, Phys. Chem. Chem. Phys., **20**, 6657, (2018). https://doi.org/10.1039/c8cp00026c

116. M. Campetella, 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). https://doi.org/10.1021/acs.jpcb.7b12455

115. 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). https://doi.org/10.1016/j.molliq.2017.11.152

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114. 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). https://doi.org/10.1021/acs.inorgchem.7b01900

113. A. Ciavardini, S. Fornarini, A. Dalla Cort, S. Piccirillo, D. Scuderi, and E. Bodo* *Experimental and Computational Investigation of Salophen-Zn Gas Phase Complexes with Cations: A Source of Possible Interference in Anionic Recognition*, J Phys. Chem. A **121**, 7042-7050, (2017). https://doi.org/10.1021/acs.jpca.7b05825

112. M. Montagna, R. Spezia and E. Bodo*, *Structural and energetic properties of La^{3+} in water/DMSO mixtures*, J. Mol. Struct. **1148**, 381-387, (2017). https://doi.org/10.1016/j.molstruc.2017.07.068

111. M. Campetella, 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). https://doi.org/10.1039/c7cp01050h

110. A. Ciavardini, A. Dalla Cort, S. Fornarini, D. Scuderi, A. Giardini, G. Forte, E. Bodo* *Adenosine monophosphate recognition by zinc-salophen complexes: IRMPD spectroscopy and quantum modeling study*, J. Mol. Spectr., **335**, 108-116, (2017). https://doi.org/10.1016/j.jms.2017.02.014

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109. 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). https://doi.org/10.1002/chem.201603298

108. Allegretti, M., Aramini A., Barile F., Bodo E., Daidone I., Guzzo T., Mandaliti W, Nepravishta R.,f, Topai A. and Paci M. *The conformational change in the mechanism of host-guest inclusion complex of Ketoprofen in cyclodextrin : NMR spectroscopy, ab initio calculations, molecular dynamics simulations and photoreactivity.* , J. Phys. Chem. B, **120**, 10668-10678 (2016). https://doi.org/10.1021/acs.jpcb.6b07913

107. M. Campetella, E. Bodo*, M. Montagna, S. De Santis and L. Gontrani *Theoretical study of ionic liquids based on the cholinium cation. Ab initio simulations of their condensed phases*, J. Chem. Phys. **144**, 104504 (2016). https://doi.org/10.1063/1.4943197

106. M. Montagna, Y. Jeanvoine, R. Spezia and E. Bodo* *Structure, Stability and Electronic Properties of DMSO and DMF clusters containing Th^{4+}*. J. Phys. Chem. A **120**, 4778-4788 (2016). https://doi.org/10.1021/acs.jpca.5b12007

105. 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). https://doi.org/10.1021/acs.jpcb.5b06317
104. 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). https://doi.org/10.1021/acs.jpcb.5b06387
103. M. Campetella, E. Bodo*, R. Caminiti, A. Martino, F. D'Apuzzo, S. Lupi and L. Gontrani *Interaction and dynamics of ionic liquids based on Choline and amino-acids anions.* J. Chem. Phys., **142**, 234502 (2015). https://doi.org/10.1063/1.4922442

102. E. Bodo, M. Chiricotto, R. Spezia, *Structural, Energetic and Electronic Properties of La(III)-DMSO Clusters*, J. Phys. Chem. A, **118**, 11602-11611, (2014)
101. 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).
100. M. P. Donzello, G. De Mori, D. Futur, Z. Fu, M. L. Astolfi, C. Rizzoli, C. Ercolani,a L. Mannina, E. Bodo, and K. M. Kadish, UV-Visible, *Experimental and DFT/Time-Dependent DFT Studies on Neutral and One-Electron-Reduced Quinoxaline and Pyrazine Precursors and Their Mononuclear (Pd^{II}, Pt^{II}) Derivatives*, Eur. J. Inorg. Chem., **2014**, 3572-3581, (2014).
99. 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).
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