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

PUBLICATION LIST

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, (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 NH2OH+ 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

---

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

---

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

---

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

---

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

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

---

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

---

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

---

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).

98. E. Bodo, S. Mangialardo, F. Capitani, L. Gontrani, F. Leonelli, and P. Postorino *Interaction of a Long Alkyl Chain Protic Ionic Liquid and Water*, J. Phys. Chem., **140**, 204503, (2014).

97. C. Battocchio, I. Fratoddi, L. Fontana, E. Bodo, F. Porcaro, C. Meneghini, I. Pisc, S. Nappini, S. Mobilio, M.V. Russo, G. Polzonetti *Silver nanoparticles linked by Pt-containing organometallic dithiol bridge: study on local structure and interface by XAFS and SR-XPS*, Phys. Chem. Chem. Phys. **16** 11719-28, (2014)

---

96. S. Piccirillo, A. Ciavardini, E. Bodo, F. Rondino, D. Scuderi, V. Steinmetz, A. Paladini, *Probing the competition among different coordination motifs in metal - ciprofloxacin complexes through IRMPD spectroscopy and DFT calculations* Inorg. Chem., **52**, 103-112, (2013).

95. M. Alagia, E. Bodo*, P. Decleva, S.Falcinelli, A. Ponzi, R. Richter and S. Stranges* *Soft x-ray absorption spectrum of the allyl free radical*, Phys. Chem. Chem. Phys., **15**, 1310-1318, (2013).

94. A. Ruggi, R. Cacciapaglia, S. Di Stefano, E. Bodo, F. Ugozzoli, *Naphthalenophane Formaldehyde Acetals as Candidate Structures for the Generation of Dynamic Libraries via Transacetalation Processes*, Tetrahedron, **69**, 2767-2774, (2013).

93. M. Campetella, L. Gontrani, E. Bodo, F. Ceccacci, F. C. Marincola, R. Caminiti *Conformational Isomerisms and Nano-Aggregation in Substituted Alkylammonium Nitrates Ionic Liquids: an X-ray and Computational Study of 2-OMeEAN* J. Chem. Phys. **138**, 184506, (2013)

92. E. Bodo*, S. Mangialardo, P. Postorino, A. Sferrazza, and R. Caminiti, *A Prototypical Ionic Liquid Explored by Ab-initio Molecular Dynamics*, J. Chem. Phys. **139**, 144309 (2013)

---

91. E. Bodo, A. Ciavardini, A. Giardini, A. Paladini, S. Piccirillo, F. Rondino, D. Scuderi, *Infrared Multiple Photon Dissociation Spectroscopy of Ciprofloxacin: Investigation of the Protonation Site*, Chem. Phys., **398**, 124 (2012).

90. I. Fratoddi, E. S. Bronze-Uhle, A. Batagin-Neto, D. M. Fernandes, E. Bodo, C. Battocchio, I. Venditti, F. Decker, M.V. Russo, G. Polzonetti, C. F. O. Graeff, *Structural Changes of conjugated Pt-containing polymetallaynes exposed to gammaray radiation doses*, J. Phys. Chem C, **116**, 8768 (2012)

89. E. Bodo*, S. Mangialardo, F. Ramondo, F. Ceccacci, and P. Postorino, *Unravelling the Structure of Protic Ionic Liquids with Theoretical and experimental methods: Ethyl-, Propyl- and Butyl Ammonium Nitrate Explored by Raman spectroscopy and DFT calculations* J. Phys. Chem. B, **116**, 13878-13888 (2012).

88. L. Gontrani, E. Bodo*, A. Triolo, F. Leonelli, P. D'Angelo, V. Migliorati, R. Caminiti. *The interpretation of diffraction patterns of Protic Ionic Liquids: a challenging task for classical molecular dynamics simulations*, J. Phys. Chem. B, **116**, 13024-13032 (2012)

---

87. O. Lanzalunga, L. Mandolini, S. Di Stefano, M. Mazzonna, E. Bodo, *Photoinversion of Sulfoxides as a Source of Diversity in Dynamic Combinatorial Chemistry* Org. Lett., **13**; 142-145, (2011).

86. A. Batagin-Neto, E. Bronze-Uhle, D. Fernandes, I. Fratoddi, I. Venditti, F. Decker, E. Bodo, M.-V. Russo, C. Graeff, *Optical Behavior of Conjugated Pt-containing Polymetallaynes Exposed to Gamma-ray Radiation Doses*, J. Phys Chem C, **115**, 8047 (2011).

85. P. D'angelo, A. Zitolo, V. Migliorati, E. Bodo, G. Aquilanti, J.-L. Hazemann, D. Testemale, G. Mancini, R. Caminiti, *X-Ray absorption spectroscopy investigation of 1-alkyl-3-methylimidazolium bromide salts* J. Chem. Phys., **135**, 074505 (2011).

84. P. Zhang, A. Dalgarno, R. Cotê, E. Bodo*, *Charge exchange in collisions of Beryllium with its ion*. Phys. Chem. Chem. Phys., **13**, 19026-19035 (2011).

83. M.-P. Donzello, G. De Mori, C. Ercolani, E. Bodo, L. Mannina, D. Capitani, C. Rizzoli, L. Gontrani, G. Aquilanti, K. M. Kadish, P. D'Angelo, *Structural Flexibility and Role of Vicinal 2-Thienyl Rings in 2,3-Dicyano-5,6-di(2-thienyl)-1,4-pyrazine, [(CN)2Th2Pyz], its Palladium(II) Complex [(CN)2Th2Pyz(PdCl2)2] and the Related Pentametallic Pyrazinoporphyrazines [(PdCl2)4Th8TPyzPzM] (M = MgII(H2O), ZnII)*, Inorg. Chem. **50**, 12116-12125, (2011).

82. E. Bodo*, P. Postorino, S. Mangialardo, G. Piacente, F. Ramondo, F. Bosi, P. Ballirano, and R. Caminiti, *The Structure of the Molten Salt Methyl Ammonium Nitrate Explored by Experiments and Theory*, J. Phys. Chem. B, **115** (2011), 13149-13161.

81. E. Bodo*, M. Chiricotto and R. Caminiti, *The Structure of Geminal Imidazolium Bis(trifluoromethanesulfonyl)imide Dicationic Ionic Liquids: a Theoretical Study of the Liquid Phase*, J. Phys. Chem. B **115**, 14341-14347, (2011).

---

80. E. Bodo*, L. Gontrani, A. Triolo, and R. Caminiti *Structural determination of Ionic Liquids with theoretical methods: C_8mimBr and C_8mimCl. Strength and weakness of current force fields.* J. Phys. Chem. Lett. **1**, 1095-1100 (2010).

79. E. Bodo* and G. Lanaro *Theoretical treatment of the electronic excited states of the DMSO molecule: a challenge for current theoretical method*, Chem. Phys **337**, (2010), 136-141.

78. E. Bodo* and R. Caminiti The Structure of Geminal Imidazolium *Bis-(trifluoromethyl-sulfonyl)amide Ionic Liquids: a Theoretical Study of the Gas Phase Ionic Complexes*, J. Phys. Chem. A, **114**, 12506, (2010)

77. E. Bodo*, L. Gontrani, R. Caminiti, N. V. Plechkova, K. R. Seddon and A. Triolo, *Structural properties of 1-alkyl-3-methylimidazolium bis{(trifluoromethyl)sulfonyl}amide ionic liquids:X-ray Diffraction Data and Molecular Dynamics Simulations* J. Phys. Chem. B, **114**, 16398, (2010).

---

76. E. Coccia, E. Bodo, and F. A. Gianturco *Size-dependent solvation of p-H2 in 4He clusters: A quantum Monte Carlo analysis* J. Chem. Phys. **130**, 094906 (2009)
75. M. Wernli, E. Scifoni, E. Bodo, F.A. Gianturco *A quantum modeling of the chemistry of LiH^+ with He from ab initio calculations: Ionic reactions in He nanodroplets* Int. J. of Mass Spectr., **280**, 57, (2009)
74. M. Wernli, D. Caruso, E. Bodo, and F. A. Gianturco *Computing a three-dimensional electronic energy manifold for the* $\mathrm{LiH} + \mathrm{H} \rightleftharpoons \mathrm{Li} + \mathrm{H}_2$ *chemical reaction* J. Phys. Chem A, **113**, 1121, (2009)
73. S. Bovino, E. Coccia, E. Bodo, D. Lopez-Duraán and F. A. Gianturco *Spin-driven structural effects in alkali doped* ^{4}*He clusters from quantum calculations*, J. Chem. Phys. **130**, 224903 (2009)
72. P. Zhang, E. Bodo, and A. Dalgarno *Near Resonance Charge Exchange in Ion-Atom Collisions of Lithium Isotopes* J. Phys. Chem. A **113** 15085 (2009).
71. E. Bodo*, *Low and Ultra-low energy chemical processes involving ions* Phys. Scripta., **80**, 048117, (2009)

---

70. E. Bodo* P. Zhang, A. Dalgarno, *Ultra-cold ion-atom collisions: near resonant charge exchange.* New J. Phys., **10**, 033024 (2008)
69. E. Coccia, F. Marinetti, E. Bodo, and F.A. Gianturco *Anionic microsolvation in helium droplets:* $(OH^-)(He)_N$ *structures from classical and quantum calculations,* J. Chem . Phys., **128,** 134511 (2008).
68. S. Bovino, E. Bodo, and F.A. Gianturco *Ultralow energy vibrational quenching in ionic collisions: Isotope effects in* $Li^+ + D_2$ *encounters by.* Phys Rev. A, **77**, 042716 (2008)
67. E. Coccia, E. Bodo and F. A. Gianturco, *Nanoscopic phase changes in doped* ^{4}*He droplets.* Eur. Phys. Lett., **82,** 23001, (2008)
66. L. González-Sánchez, E. Bodo, E. Yurtsever, F.A. Gianturco, *Quenching efficiency of hot polar molecules by He buffer gas at ultralow energies: quantum results for MgH and LiH rotations.* Eur Phys J. D **48**, 75 (2008)
65. F. Leonelli, M. Capuzzi, E. Bodo, P. Passacantilli and G. Piancatelli, *Synthesis of New 2-Phosphono-alpha-D-Glycoside derivatives by Stereoselective Oxa-Michael Addition to D-Galacto Derived Enone* CARBOHYD RES, **343**, 1133, (2008)
64. S. Bovino, E. Bodo, E. Yurtsever, and F.A. Gianturco, *Vibrational cooling of spin-stretched dimer states by He buffer gas: Quantum calculations for* $Li_2(a^3\Sigma_u^+)$ *at ultralow energies*, J. Chem. Phys, **128,** 224312, (2008)
63. L. González-Sńchez, M. Tacconi, E. Bodo, and F.A. Gianturco, *Ionic interactions and collision dynamics in cold traps: rotational quenching of* $OH^-(^1\Sigma^+)$ *by Rb(*^{2}*S)*, Eur. Phys. J. D, **49**, 85-92, (2008)
62. E. Coccia, F. Marinetti, E. Bodo and F. A. Gianturco, *Chemical solutions in a quantum solvent: anionic "electrolytes" in* ^{4}*He nanodroplets,* ChemPhysChem, **9**, 1323-1330, (2008)
61. D. López-Dúran, E. Bodo, F. A. Gianturco, *ASPIN: an all spin scattering code for atom molecule rovibrationally inelastic cross sections* Comp. Phys. Comm. **179**, 821 (2008)
60. F. Marinetti, E. Bodo, E. Yurtsever, F. A. Gianturco, *Energetics and structures of charged helium clusters: comparing stabilities of dimer and trimer cationic cores*, ChemPhysChem **9**, 2618, (2008)

---

59. F. Marinetti, E. Bodo and F. A. Gianturco, *Microsolvation of an ionic Dopant in small* ^{4}He *clusters:* $OH^+(^3\Sigma)(^4He)_n$ *via Genetic Algorithm Optimizations.* ChemPhysChem, **8**, 93, (2007)
58. E. Bodo, F.A. Gianturco, *Quenching of vibrationally excited molecules by ultracold collisions with ions: Controlling the scattering via changes of internal states* Eur. Phys. Lett.**77,** 33001 (2007)
57. M. Tacconi, E. Bodo, F.A. Gianturco, *Sympathetic cooling of* NH*(*$X^3\Sigma$*) molecules by* Rb *and* Cs *atoms at ultralow energies* Phys. Rev. A, **75,** 012708, (2007)

56. E. Coccia, E. Bodo, F. Marinetti, F. A. Gianturco, E. Yildrim, M. Yurtsever and E. Yurtsever, *Bosonic helium droplets with cationic impurities: Onset of electrostriction and snowball effects from quantum calculations,* J. Chem. Phys., **126**, 124319, (2007).

55. M. Tacconi, E. Bodo and F.A. Gianturco, *Interaction of* NH$(^3X\Sigma^-)$ *with* Rb *and* Cs *atoms: similarities and differences from an highly correlated ab initio study* Theor. Chem. Acc., **117**, 649-662, (2007)

54. E. Yurtsever, E. Yildirim, M. Yurtsever, E. Bodo, and F. A. Gianturco, *Solvation of* K^+ *in Helium droplets* , Eur. Phys. J. D, **43**, 105, (2007)

53. L. González-Sánchez, E. Bodo and F.A. Gianturco, *Quenching of molecular ions by* He *buffer loading at ultralow energies: rotational cooling of* $OH^+(^3\Sigma^-)$ *from quantum calculations,* Eur Phys. J. D**, 44**, 65, (2007)

52. F. Marinetti, E. Coccia, E. Bodo F. A. Gianturco, E. Yurtsever, M. Yurtsever, E. Yildirim, *Bosonic Helium Clusters Doped by Alkali Cations: Interaction Forces and Analysis of Their Most Stable Structures*, Theor. Chem. Acc., **118**, 53, (2007)

51. M. Tacconi, L. Gonzalez-Sanchez, E. Bodo, F.A. Gianturco, *Collisions of* NH$(^3\Sigma^-)$ *with* Rb *and* Cs *at ultralow energies*: *A quantum study of rotational cooling efficiency,* Phys. Rev. A, **76,** 032702 (2007)

50. M. Wernli, E. Bodo and F.A. Gianturco, *Rotational cooling efficiency upon molecular ionization: the case of* Li_2 $(a^3\Sigma_u^+)$ *and* Li_2^+ $(X^2\Sigma_g^+)$ *interacting with* ^{4}*He,* Eur. Phys. J. D, **45**, 267-272, (2007)

49. S. Bovino, E. Bodo, and F.A. Gianturco, *Collisional quenching at ultralow energies: Controlling efficiency with internal state selection,* J. Chem . Phys., **127**, 224303 (2007).

48. B. C. Shepler, B. H. Yang, T. J. Dhilip Kumar, P. C. Stancil, J. M. Bowman, N. Balakrishnan, P. Zhang, E. Bodo, and A. Dalgarno, *Low energy H+CO scattering revisited: CO rotational excitation with new potential surfaces,* Astronomy and Astrophysics, **475** L15-L18, (2007).

47. F. Marinetti, Ll. Uranga-Pina, E. Coccia, D. López-Durán, E. Bodo, and F. A. Gianturco, *Microsolvation of cationic dimers in* ^{4}*He droplets: geometries of* A_2^+ $(He)_N$ *(*A = Li, Na, K*) from optimized energies.,* J. Phys. Chem. A, **111**, 12289, (2007)

46. L. González-Sánchez, E. Bodo, F. A. Gianturco, *Collisional quenching of rotations in lithium dimers by ultracold helium: the* Li_2 $(a^3\Sigma_u^+)$ *and* Li_2 $(X^1\Sigma_g^+)$ *targets,* J. Chem . Phys., **127,** 244315 (2007)

45. E. Bodo, E. Coccia, D. López-Durán, and F. A. Gianturco, *Ionic dopants in* He *droplets: cluster energies from a variational and diffusion Monte Carlo approach,* Phys. Scripta., **76**, C104-C110, (2007)

---

44. F. Sebastianelli, I. Baccarelli, E. Bodo, C. Di Paola, F. A. Gianturco and M. Yurtsever, *Microsolvation of* Li^+ *in Bosonic Helium Clusters. I: Many body effects on the structures of the small aggregates*, Computational Materials Science **35**, 261-267, (2006).

43. E. Bodo, M. Lara and F. A. Gianturco, *Isotopic replacement in ionic systems: the* $^4\mathrm{He}_2^+ + {}^3\mathrm{He} \longrightarrow {}^3\mathrm{He}^4\mathrm{He}^+ + {}^4\mathrm{He}$ *reaction,* J. Chem. Phys. **124**, 044308 (2006).

42. E. Bodo, E. Yurtsever, M. Yurtsever and F. A. Gianturco, *Ionic dimers in He droplets: interactions potentials for* Li_2^+*-He,* Na_2^+ *-He and* K_2^+ *-He and stability of the smaller clusters,* J. Chem. Phys. **124**, 074320 (2006).

41. L. González-Sánchez, E. Bodo, F. A. Gianturco, *Quantum scattering of OH*$(X^2\Pi)$ *with He*(^1S)*: propensity features in rotational relaxation at ultralow energies,* Phys. Rev. A, **73,** 022703, (2006)

40. E. Bodo and F. A. Gianturco, *Ultra-low energy behavior of an ionic replacement reaction* $^4\mathrm{He}_2^+ + {}^3\mathrm{He} \longrightarrow {}^3\mathrm{He}^4\mathrm{He}^+ + {}^4\mathrm{He}$, Phys. Rev. A, **73,** 032702, (2006).

39. E. Bodo and F. A. Gianturco, *Vibrational quenching at ultralow energies: calculations of the* $Li_2(^1\Sigma_g^+;\nu \gg 0)$*+He superelastic scattering cross sections,* Phys. Rev. A, **73**, 052715, (2006)

38. E. Bodo, F.A. Gianturco, *Collisional Quenching of molecular rovibrational energy by He buffer loading at ultralow energies* Int. Rev. Phys. Chem. **25,** 313, (2006).

37. L. Gonzalez-Sanchez, F. Marinetti, E. Bodo, F.A. Gianturco, OH^-*(*$X^1\Sigma^+$*) Collisions with* ^{4}He*(1S) at vanishing energies: a quantum analysis of rotational quenching efficiency*, J. Phys. B, **39**, S1203, (2006).

36. F. Marinetti, E. Bodo and F. A. Gianturco, *Ionic OH as dopant of heliun droplets: ab initio potential energy surfaces for* $OH^+(^3\Sigma)$-^4He, $OH^-(^1\Sigma)$-^4He *and stable structures of their smaller clusters,* J. Theo. & Comput. Chem. **5,** 543 (2006).

35. C. Di Paola, E. Bodo and F.A. Gianturco, *Adaptive clustering of a quantum solvent: the* LiH^+ *impurity in bosonic helium from stochastic calculations*, Eur. Phys. J. D. **40,** 377 - 385, (2006).

---

34. E. Bodo, F.A. Gianturco, and E. Yurtsever, *The Weak* Li_2-He *Interaction Revisited: a Combined Ab-Initio and Empirical Modelling*, J. Low. Temp. Phys., **138**, 259, (2005).

33. C. Sanz, E. Bodo and F. A. Gianturco, *Energetics and Structure of the Bound States in a Lithium Complex: The* LiH_2^+ *Electronic Ground State* Chem. Phys., **314**, 135, (2005).

32. E. Bodo, F. Sebastianelli, F. A. Gianturco and I. Pino, *Microsolvation of* LiH^+ *in Helium Clusters: many-body effects and additivity models for the interaction forces*, J. Phys. Chem. A, **109**, 4252, (2005).

31. J. Sabin Del Valle, E. Bodo, and F.A. Gianturco, *Rotational cooling of molecular gases by positron impact at vanishing collision energies*, J. Phys. B, **38,** 2069, (2005).

30. C. Di Paola, F. Sebastianelli, E. Bodo, I. Baccarelli, F. A. Gianturco and M. Yurtsever, *Microsolvation of* Li^+ *in Small He Clusters.* Li^+He_n *Species from Classical and Quantum Calculations*; J. Chem. Theory and Comput., **1,** 1045, (2005).

29. E. Scifoni, E. Bodo, F.A. Gianturco, *Ionic Reactions in He nanodroplets: the LiHHe*$^+$ *complex and its possible energy pathways into products from ab-initio calculations*, J. Chem. Phys., **122,** 224312, (2005)

28. E. Bodo , F. A. Gianturco , E. Yurtsever, M. Yurtsever, *Neutral and ionic dopants in helium clusters: interaction forces for the* $Li_2(a^3\Sigma_u^+)$He *and* $Li^+(X^2\Sigma_g^+)$He *complexes,* Mol. Phys., **103,** 3223, (2005).

---

27. S. Telega, E. Bodo and F. A. Gianturco, *Rotationally inelastic collision of electrons with* H_2 *and* N_2 *molecules: converged space-frame calculations at low energies,* Eur. Phys. J. D, **29**, 357, (2004).

26. E. Bodo F. A. Gianturco F. Sebastianelli E. Yurtsever M. Yurtsever, *Rotational cooling of* $Li_2(^1\Sigma_g^+)$ *molecules by ultracold collisions with an* He *gas buffer,* Theor. Chem. Acc., **112**, 263, (2005).

25. E. Bodo F. A. Gianturco F. Sebastianelli E. Yurtsever M. Yurtsever, *Ab initio quantum dynamics with very weak Van der Waals interactions: structure and stability of small* $Li_2(^1\Sigma_g^+) - ^4 He$ *clusters,* J. Chem. Phys., **120**, 9160, (2004).

24. E. Bodo and F. A. Gianturco, *Features of chemical reactions at vanishing kinetic energy: the presence of internally hot reagents,* Eur. Phys. J. D, **31,** 423, (2004)

23. E. Bodo, F. A. Gianturco, N. Balakrishnan and A. Dalgarno, *Chemical reactions in the limit of zero kinetic energy: virtual; states and Ramsauer minima in* $F + H_2 \rightarrow HF + H$, J. Phys. B, **37**, 1, (2004).

22. E. Scifoni, E. Bodo and F. A. Gianturco, *Charged cores in ionized* ^{4}*He clusters III: a quantum model for the collisional relaxation dynamics*, Eur. Phys. J. D, **30**, 363, (2004)

---

21. R. Martinazzo, E. Bodo, and F. A. Gianturco, *A modified Variable-Phase algorithm for multichannel scattering with long-range potentials,* Comp. Phys. Comm., **151**, 187, (2003)

20. R. Martinazzo, E. Bodo, F. A. Gianturco and M. Raimondi, *Three-dimensional reactive surfaces for the* LiH_2^+ *system: an analysis of accurate ab-initio results,* Chem. Phys., **287**, 335, (2003).

19. E. Bodo, F. A. Gianturco, and R. Martinazzo, *The gas-phase lithium chemistry in the early universe: elementary processes, interaction forces and quantum dynamics,* Phys. Rep., **384,** 85, (2003).

18. R. Martinazzo, G. F. Tantardini, E. Bodo and F. A. Gianturco, *Accurate potential energy surfaces for the study of lithium-hydrogen ionic reactions,* J. Chem. Phys. , **119**, 11241, (2003).

17. E. Bodo, F. A. Gianturco, *Collisional Cooling of Polar Diatomics in* ^3He *and* ^4He *Buffer Gas: A Quantum Calculation at Ultralow Energies*, J. Phys. Chem. A., **107**, 7328, (2003).

---

16. E. Bodo, F. A. Gianturco, and A. Dalgarno, *Quenching of vibrationally excited CO(*$\nu = 2$*) molecules by ultra-cold collisions with* ^4He *atoms,* Chem. Phys. Lett., **353**, 1, (2002).

15. E. Bodo, A. Dalgarno, and F. A. Gianturco, *F+D_2 reaction at ultra-low temperatures,* J. Chem. Phys., **116**, 9222, (2002).
14. C. Cecchi-pestellini, E. Bodo, N. Balakhrishnan, and A. Dalgarno. *Rotational and vibrational excitation of CO molecules by collisions with He atoms.* ApJ, **571**, 1015, (2002),
13. E. Bodo, A. Dalgarno, and F. A. Gianturco. *F+D_2 reaction at ultra-low temperatures, the effect of rotational excitation,* J. Phys. B, **35**, 2391, (2002).
12. M. Satta, E. Bodo, R. Martinazzo and F.A. Gianturco, *Photoexcitation of LiH_2^+ from selected initial states: a time-dependent model,* J. Chem. Phys., **117**, 177, (2002).
11. E. Bodo, E. Scifoni, F. Sebastianelli, F.A. Gianturco, and A. Dalgarno, *Rotational quenching in ionic systems at ultra-cold temperatures,* Phys. Rev. Lett., **89** , (2002).

---

10. E. Bodo, F. A. Gianturco, R. Martinazzo, and M. Raimondi, *Computed orientational anisotropy and vibrational couplings for the LiH-H interaction potential,* Eur. Phys. J. D, **15**, 321, (2001).
9. E. Bodo, F. A. Gianturco, R. Martinazzo, and M. Raimondi, *Possible reaction paths in the LiH_2^+ chemistry: a computational analysis of the interaction forces,* Chem. Phys., **271,** 309, (2001).
8. E. Bodo, F. A. Gianturco, and R. Martinazzo, *Reactive behavior of the LiH_2^+ system I: Evaluation of the lower lying potentials for the collinear geometries,* J. Phys. Chem. A, **105**, 10986, (2001).
7. E. Bodo, F. A. Gianturco, and R. Martinazzo, *Reactive behavior of the LiH_2^+ system II: Collision induced dissociation and collinear reaction dynamics of $\mathrm{LiH}^+ + \mathrm{H}$ from quantum time dependent calculations,* J. Phys. Chem. A, **105**, 10994, (2001).
6. R. Martinazzo, A. Famulari, M. Raimondi, E. Bodo, and F.A. Gianturco, *A multireference valence bond approach to electronic excited states,* J. Chem. Phys., **115**, 2917, (2001).

---

5. E. Bodo, F. A. Gianturco, R. Martinazzo, A. Forni, A. Famulari, and M. Raimondi, *Spatial energetics of protonated LiH: Lower-lying potential energi surfaces from valence bond calculations,*J. Phys. Chem. A, **104**, 11972, (2000).
4. E. Bodo, F. A. Gianturco, R. Martinazzo, F. Paesani, and M. Raimondi, *Testing van der waals interactions with quantum dynamics: repulsive anisotropy and well depth in LiH-He system,* J. Chem. Phys., **113**, 11071, (2000).
3. E. Bodo, F. A. Gianturco, F. Paesani, *Testing intermolecular potentials with scattering experiments: He-CO rotationally inelastic scattering,* Zeit. Phys. Chem, **214**, 1013, (2000).

---

2. E. Bodo, E. Buonomo, F.A. Gianturco, S. Kumar, A. Famulari, M. Raimondi, and M. Sironi, *Interaction anisotropy and quantum dynamics for vibrationally inelastic collision of LiH($^1\Sigma^+$) with He(^1S)*, Chem. Phys., **237**, 315, (1998).
1. E. Bodo, S. Kumar, F. A. Gianturco, A. Famulari, M. Raimondi, and M. Sironi, *Vibrational heating efficiency of LiH($^1\Sigma^+$) molecules in collision with He(^1S) atoms*, J. Phys. Chem. A, **102**, 9390, (1998).

Books Chapters

1. A. Mariani, L. Engelbrecht, A. Le Donne, F. Mocci, E. Bodo and S. Passerini *Disclosing the hierarchical structure of ionic liquid mixtures by multiscale computational methods* in *Theoretical and Computational Approaches to Predicting Ionic Liquid Properties*, A. Joseph and S. Mathew eds., Elsevier, Amsterdam, Netherlands, (2021)
2. S. Mangialardo, L. Baldassarre, E. Bodo, and P. Postorino, *Raman Spectroscopy in Ionic Liquids Under Variable Thermodynamic and Environmental Conditions.* in *The Structure of Ionic Liquids* R. Caminiti and L. Gontrani (Eds), Soft and Biological Matter, Elsevier, Amsterdam, Netherlands, (2013)
3. E. Bodo and V. Migliorati *Theoretical Description of Ionic Liquids* in *The Structure of Ionic Liquids* R. Caminiti and L. Gontrani eds., Soft and Biological Matter, Elsevier, Amsterdam, Netherlands, (2013)
4. E. Bodo and V. Migliorati (2011). *Theoretical Description of Ionic Liquids* in *Ionic Liquids - Classes and Properties*, Scott T. Handy eds., InTech, (2011)
5. E. Coccia, E. Bodo, F. Marinetti and F.A. Gianturco E. Yurtsever, M. Yurtsever, E. Yildirim, *Quantum structuring of ^{4}He Atoms around Ionic Dopants: energetics of Li^+, Na^+ and K^+ from Stochastic Calculations.* in *Latest Advances in Atomic Cluster Collisions: Structure and Dynamics from the Nuclear to the Biological Scale*, Imperial College Press.