Enrico Bodo

List of Publications by Citations

148 papers	2,711 citations	30 h-index	40 g-index
153 ext. papers	2,869 ext. citations	3.3 avg, IF	5.31 L-index

#	Paper	IF	Citations
148	F+D2 reaction at ultracold temperatures. *Journal of Chemical Physics*, **2002**, 116, 9222-9227	3.9	94
147	Structural properties of 1-alkyl-3-methylimidazolium bis{(trifluoromethyl)sulfonyl}amide ionic liquids: X-ray diffraction data and molecular dynamics simulations. *Journal of Physical Chemistry B*, **2010**, 114, 16398-407	3.4	92
146	Unravelling the structure of protic ionic liquids with theoretical and experimental methods: ethyl-, propyl- and butylammonium nitrate explored by Raman spectroscopy and DFT calculations. *Journal of Physical Chemistry B*, **2012**, 116, 13878-88	3.4	74
145	Chemical reactions in the limit of zero kinetic energy: virtual states and Ramsauer minima inF + H2HF + H. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2004**, 37, 3641-3648	1.3	71
144	The gas-phase lithium chemistry in the early universe: elementary processes, interaction forces and quantum dynamics. *Physics Reports*, **2003**, 384, 85-119	27.7	66
143	Accurate potential energy surfaces for the study of lithiumhydrogen ionic reactions. *Journal of Chemical Physics*, **2003**, 119, 11241-11248	3.9	61
142	The interpretation of diffraction patterns of two prototypical protic ionic liquids: a challenging task for classical molecular dynamics simulations. *Journal of Physical Chemistry B*, **2012**, 116, 13024-32	3.4	59
141	A modified Variable-Phase algorithm for multichannel scattering with long-range potentials. *Computer Physics Communications*, **2003**, 151, 187-198	4.2	52
140	Structure of the molten salt methyl ammonium nitrate explored by experiments and theory. *Journal of Physical Chemistry B*, **2011**, 115, 13149-61	3.4	49
139	Bosonic helium droplets with cationic impurities: onset of electrostriction and snowball effects from quantum calculations. *Journal of Chemical Physics*, **2007**, 126, 124319	3.9	49
138	Rotational and Vibrational Excitation of CO Molecules by Collisions with4He Atoms. *Astrophysical Journal*, **2002**, 571, 1015-1020	4.7	44
137	Interaction and dynamics of ionic liquids based on choline and amino acid anions. *Journal of Chemical Physics*, **2015**, 142, 234502	3.9	43
136	Collisional quenching of molecular ro-vibrational energy by He buffer loading at ultralow energies. *International Reviews in Physical Chemistry*, **2006**, 25, 313-351	7	43
135	Possible reaction paths in the LiH+2 chemistry: a computational analysis of the interaction forces. *Chemical Physics*, **2001**, 271, 309-321	2.3	42
134	The soft X-ray absorption spectrum of the allyl free radical. *Physical Chemistry Chemical Physics*, **2013**, 15, 1310-8	3.6	41
133	Amino acid anions in organic ionic compounds. An ab initio study of selected ion pairs. *Journal of Physical Chemistry B*, **2014**, 118, 2471-86	3.4	40
132	Computing a three-dimensional electronic energy manifold for the LiH + H Li + H2 chemical reaction. *Journal of Physical Chemistry A*, **2009**, 113, 1121-8	2.8	39

131	ASPIN: An all spin scattering code for atom□molecule rovibrationally inelastic cross sections. *Computer Physics Communications*, **2008**, 179, 821-838	4.2	36
130	Three-dimensional reactive surfaces for the LiH2+ system: an analysis of accurate ab initio results. *Chemical Physics*, **2003**, 287, 335-348	2.3	36
129	Structure of geminal imidazolium bis(trifluoromethylsulfonyl)imide dicationic ionic liquids: a theoretical study of the liquid phase. *Journal of Physical Chemistry B*, **2011**, 115, 14341-7	3.4	35
128	A prototypical ionic liquid explored by ab initio molecular dynamics and Raman spectroscopy. *Journal of Chemical Physics*, **2013**, 139, 144309	3.9	34
127	Interaction of a long alkyl chain protic ionic liquid and water. *Journal of Chemical Physics*, **2014**, 140, 204503	3.9	32
126	Ultra-cold ion□atom collisions: near resonant charge exchange. *New Journal of Physics*, **2008**, 10, 033024	2.9	32
125	Structural Determination of Ionic Liquids with Theoretical Methods: C8mimBr and C8mimCl. Strength and Weakness of Current Force Fields. *Journal of Physical Chemistry Letters*, **2010**, 1, 1095-1100	6.4	31
124	Microsolvation of Li(+) in Small He Clusters. Li(+)Hen Species from Classical and Quantum Calculations. *Journal of Chemical Theory and Computation*, **2005**, 1, 1045-54	6.4	31
123	Hydrogen Bonding Features in Cholinium-Based Protic Ionic Liquids from Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2018**, 122, 2635-2645	3.4	30
122	Energetics and structure of the bound states in a lithium complex: The (LiH2)+ electronic ground state. *Chemical Physics*, **2005**, 314, 135-142	2.3	30
121	Spatial Energetics of Protonated LiH: Lower-Lying Potential Energy Surfaces from Valence Bond Calculations. *Journal of Physical Chemistry A*, **2000**, 104, 11972-11982	2.8	30
120	Reactive Behavior of the [LiH2]+ System I. Evaluation of the Lower-lying Electronic Potentials for the Collinear Geometries. *Journal of Physical Chemistry A*, **2001**, 105, 10986-10993	2.8	30
119	Theoretical study of ionic liquids based on the cholinium cation. Ab initio simulations of their condensed phases. *Journal of Chemical Physics*, **2016**, 144, 104504	3.9	30
118	X-Ray absorption spectroscopy investigation of 1-alkyl-3-methylimidazolium bromide salts. *Journal of Chemical Physics*, **2011**, 135, 074505	3.9	29
117	Low energy H+CO scattering revisited. *Astronomy and Astrophysics*, **2007**, 475, L15-L18	5.1	29
116	A multireference valence bond approach to electronic excited states. *Journal of Chemical Physics*, **2001**, 115, 2917-2925	3.9	28
115	Unexpected proton mobility in the bulk phase of cholinium-based ionic liquids: new insights from theoretical calculations. *Physical Chemistry Chemical Physics*, **2017**, 19, 11869-11880	3.6	27
114	Conformational isomerisms and nano-aggregation in substituted alkylammonium nitrates ionic liquids: an x-ray and computational study of 2-methoxyethylammonium nitrate. *Journal of Chemical Physics*, **2013**, 138, 184506	3.9	27

113	Reactive Behavior of the [LiH2]+ System II. Collision-Induced Dissociation and Collinear Reaction Dynamics of LiH++H from Quantum Time Dependent Calculations. *Journal of Physical Chemistry A*, **2001**, 105, 10994-11000	2.8	27
112	Bosonic helium clusters doped by alkali metal cations: interaction forces and analysis of their most stable structures. *Theoretical Chemistry Accounts*, **2007**, 118, 53-65	1.9	26
111	Production, formulation and antagonistic activity of the biocontrol like-yeast Aureobasidium pullulans against Penicillium expansum. *Biotechnology Letters*, **2007**, 29, 553-9	3	26
110	Silver nanoparticles linked by a Pt-containing organometallic dithiol bridge: study of local structure and interface by XAFS and SR-XPS. *Physical Chemistry Chemical Physics*, **2014**, 16, 11719-28	3.6	25
109	Spin-driven structural effects in alkali doped (4)He clusters from quantum calculations. *Journal of Chemical Physics*, **2009**, 130, 224903	3.9	25
108	The reaction of F + D2 at ultra-low temperatures: the effect of rotational excitation. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2002**, 35, 2391-2396	1.3	25
107	Quantum scattering of OH(X□2) with He(S1): Propensity features in rotational relaxation at ultralow energies. *Physical Review A*, **2006**, 73,	2.6	23
106	Rotational quenching in ionic systems at ultracold temperatures. *Physical Review Letters*, **2002**, 89, 283201	7.4	23
105	The structure of geminal imidazolium bis(trifluoromethylsulfonyl)amide ionic liquids: a theoretical study of the gas phase ionic complexes. *Journal of Physical Chemistry A*, **2010**, 114, 12506-12	2.8	22
104	Near resonance charge exchange in ion-atom collisions of lithium isotopes. *Journal of Physical Chemistry A*, **2009**, 113, 15085-91	2.8	22
103	The Weak Li2 □He Interaction Revisited: a Combined Ab-initio and Empirical Modelling.. *Journal of Low Temperature Physics*, **2005**, 138, 259-264	1.3	22
102	Ionic dopants in He droplets: cluster energies from a variational and diffusion Monte Carlo approach. *Physica Scripta*, **2007**, 76, C104-C110	2.6	21
101	Microsolvation of Li+ in bosonic helium clusters. I. Many-body effects on the structures of the small aggregates. *Computational Materials Science*, **2006**, 35, 261-267	3.2	21
100	Ab initio quantum dynamics with very weak van der Waals interactions: Structure and stability of small Li2(1Sigmag+)-(He)n clusters. *Journal of Chemical Physics*, **2004**, 120, 9160-6	3.9	21
99	Anionic microsolvation in helium droplets: OH- (He)N structures from classical and quantum calculations. *Journal of Chemical Physics*, **2008**, 128, 134511	3.9	20
98	Microsolvation of cationic dimers in 4He droplets: geometries of A+2(He)N (A=Li, Na, K) from optimized energies. *Journal of Physical Chemistry A*, **2007**, 111, 12289-94	2.8	20
97	Quenching of vibrationally excited CO(□2) molecules by ultra-cold collisions with 4He atoms. *Chemical Physics Letters*, **2002**, 353, 127-130	2.5	20
96	Nanoscopic phase changes in doped 4 He droplets. *Europhysics Letters*, **2008**, 82, 23001	1.6	19

95	Chemical solutions in a quantum solvent: anionic electrolytes in 4He nanodroplets. *ChemPhysChem*, **2008**, 9, 1323-30	3.2	19
94	Sympathetic cooling of NH(X3)molecules by Rb and Cs atoms at ultralow energies. *Physical Review A*, **2007**, 75,	2.6	19
93	Structural changes of conjugated Pt-containing polymetallaynes exposed to gamma ray radiation doses. *Journal of Physical Chemistry A*, **2012**, 116, 8768-74	2.8	18
92	Photoinversion of sulfoxides as a source of diversity in dynamic combinatorial chemistry. *Organic Letters*, **2011**, 13, 142-5	6.2	18
91	Vibrational quenching at ultralow energies: Calculations of the Li2(+1;0)+He superelastic scattering cross sections. *Physical Review A*, **2006**, 73,	2.6	18
90	Charged cores in ionized (mathsf{{^{4}He}}) clusters III: A quantum modeling for the collisional relaxation dynamics. *European Physical Journal D*, **2004**, 30, 363-368	1.3	18
89	Microsolvation of an ionic dopant in small (4)He clusters: OH(+)((3)sigma)((4)He)(N) via genetic algorithm optimizations. *ChemPhysChem*, **2007**, 8, 93-100	3.2	17
88	Ionic dimers in He droplets: interaction potentials for Li2(+)-He,Na2(+)-He, and K2(+)-He and stability of the smaller clusters. *Journal of Chemical Physics*, **2006**, 124, 74320	3.9	17
87	Features of chemical reactions at vanishing kinetic energy: the presence of internally hot reagents. *European Physical Journal D*, **2004**, 31, 423-427	1.3	17
86	Vibrational Heating Efficiency of LiH Molecules in Collision with He Atoms *Journal of Physical Chemistry A*, **1998**, 102, 9390-9398	2.8	17
85	Amino Acid Oxidation: A Combined Study of Cysteine Oxo Forms by IRMPD Spectroscopy and Simulations. *Chemistry - A European Journal*, **2016**, 22, 17239-17250	4.8	16
84	Interaction of NH(({X}^{3}{Sigma}^{-})) with Rb and Cs atoms: similarities and differences from an highly correlated ab initio study. *Theoretical Chemistry Accounts*, **2007**, 117, 649-662	1.9	16
83	Infrared multiple photon dissociation spectroscopy of ciprofloxacin: Investigation of the protonation site. *Chemical Physics*, **2012**, 398, 124-128	2.3	15
82	IONIC OH AS DOPANT OF HELIUM DROPLETS: AB INITIO POTENTIAL ENERGY SURFACES FOR OH+(3)-4He, OH-(1)-4He, AND STABLE STRUCTURES OF THEIR SMALLER CLUSTERS. *Journal of Theoretical and Computational Chemistry*, **2006**, 05, 543-564	1.8	15
81	Hydrogen Bonding as a Clustering Agent in Protic Ionic Liquids: Like-Charge vs Opposite-Charge Dimer Formation. *ACS Omega*, **2018**, 3, 10589-10600	3.9	15
80	Lanthanum(III) and Lutetium(III) in Nitrate-Based Ionic Liquids: A Theoretical Study of Their Coordination Shell. *Journal of Physical Chemistry B*, **2015**, 119, 11833-8	3.4	14
79	Optical behavior of conjugated Pt-containing polymetallaynes exposed to gamma-ray radiation doses. *Journal of Physical Chemistry B*, **2011**, 115, 8047-53	3.4	14
78	Rotationally inelastic collisions of electrons with (mathsf{H_2}) and (mathsf{N_2}) molecules: converged space-frame calculations at low energies. *European Physical Journal D*, **2004**, 29, 357-365	1.3	14

77	Computed orientational anisotropy and vibrational couplings for the LiH + H interaction potential. *European Physical Journal D*, **2001**, 15, 321-329	1.3	14
76	Conformational Change in the Mechanism of Inclusion of Ketoprofen in β-Cyclodextrin: NMR Spectroscopy, Ab Initio Calculations, Molecular Dynamics Simulations, and Photoreactivity. *Journal of Physical Chemistry B*, **2016**, 120, 10668-10678	3.4	14
75	Structural Features of Cholinium Based Protic Ionic Liquids through Molecular Dynamics. *Journal of Physical Chemistry B*, **2019**, 123, 5568-5576	3.4	13
74	Charge exchange in collisions of beryllium with its ion. *Physical Chemistry Chemical Physics*, **2011**, 13, 19026-35	3.6	13
73	Vibrational cooling of spin-stretched dimer states by He buffer gas: quantum calculations for Li2(a 3Sigma(u)+) at ultralow energies. *Journal of Chemical Physics*, **2008**, 128, 224312	3.9	13
72	Ionic interactions and collision dynamics in cold traps: rotational quenching of OH(1Σ) by Rb(2S). *European Physical Journal D*, **2008**, 49, 85-92	1.3	13
71	OH(X1Σ) collisions with4He(1S) at vanishing energies: a quantum analysis of rotational quenching efficiency. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2006**, 39, S1203-S1213	1.3	13
70	Testing van der Waals interactions with quantum dynamics: Repulsive anisotropy and well depth in the LiH+He system. *Journal of Chemical Physics*, **2000**, 113, 11071-11078	3.9	13
69	Anion recognition by uranyl-salophen derivatives as probed by infrared multiple photon dissociation spectroscopy and ab initio modeling. *Chemistry - A European Journal*, **2014**, 20, 11783-92	4.8	12
68	Quenching of molecular ions by He buffer loading at ultralow energies: rotational cooling of OH+(3Σ) from quantum calculations. *European Physical Journal D*, **2007**, 44, 65-72	1.3	12
67	Microsolvation of LiH+ in helium clusters: many-body effects and additivity models for the interaction forces. *Journal of Physical Chemistry A*, **2005**, 109, 4252-60	2.8	12
66	Adaptive clustering of a quantum solvent: the LiH+ cation in bosonic helium from stochastic calculations. *European Physical Journal D*, **2006**, 40, 377-385	1.3	12
65	Rotational cooling of Li 2 (1Σg +) molecules by ultracold collisions with a helium gas buffer. *Theoretical Chemistry Accounts*, **2004**, 112, 263	1.9	12
64	Collisional Cooling of Polar Diatomics in 3He and 4He Buffer Gas: A Quantum Calculation at Ultralow Energies *Journal of Physical Chemistry A*, **2003**, 107, 7328-7336	2.8	12
63	Cholinium amino acid-based ionic liquids. *Biophysical Reviews*, **2021**, 13, 147-160	3.7	12
62	Adenosine monophosphate recognition by zinc-salophen complexes: IRMPD spectroscopy and quantum modeling study. *Journal of Molecular Spectroscopy*, **2017**, 335, 108-116	1.3	11
61	Energetics and structures of charged helium clusters: comparing stabilities of dimer and trimer cationic cores. *ChemPhysChem*, **2008**, 9, 2618-24	3.2	11
60	Collisions of NH(3Σ)with Rb and Cs at ultralow energies: A quantum study of rotational cooling efficiency. *Physical Review A*, **2007**, 76,	2.6	11

59	Neutral and ionic dopants in helium clusters: interaction forces for the and complexes. *Molecular Physics*, **2005**, 103, 3223-3231	1.7	11
58	Superoxide Anion Disproportionation Induced by Li and H : Pathways to O Release in Li-O Batteries. *ChemPhysChem*, **2020**, 21, 2060-2067	3.2	11
57	Ultra-Fast-VUV Photoemission Study of UV Excited 2-Nitrophenol. *Journal of Physical Chemistry A*, **2019**, 123, 1295-1302	2.8	10
56	Rotational cooling efficiency upon molecular ionization: the case of Li2(a3 +) and Li2 +(X2 +) interacting with 4He. *European Physical Journal D*, **2007**, 45, 267-272	1.3	10
55	Ionic reactions in He nanodroplets: the [LiHHe]+ complex and its possible energy pathways into products from ab initio calculations. *Journal of Chemical Physics*, **2005**, 122, 224312	3.9	10
54	Structural Features of Triethylammonium Acetate through Molecular Dynamics. *Molecules*, **2020**, 25,	4.8	9
53	Probing the competition among different coordination motifs in metal-ciprofloxacin complexes through IRMPD spectroscopy and DFT calculations. *Inorganic Chemistry*, **2013**, 52, 103-12	5.1	9
52	Isomerization patterns and proton transfer in ionic liquids constituents as probed by ab-initio computation. *Journal of Molecular Liquids*, **2018**, 249, 1075-1082	6	8
51	Collisional quenching of rotations in lithium dimers by ultracold helium: the Li2(a3Sigma u+) and Li2+(X2Sigma g+) targets. *Journal of Chemical Physics*, **2007**, 127, 244315	3.9	8
50	Assessing the Structure of Protic Ionic Liquids Based on Triethylammonium and Organic Acid Anions. *Journal of Physical Chemistry B*, **2021**, 125, 2781-2792	3.4	8
49	Vibrational signatures of curcumin's chelation in copper(II) complexes: An appraisal by IRMPD spectroscopy. *Journal of Chemical Physics*, **2019**, 150, 165101	3.9	7
48	Ab Initio Molecular Dynamics Study of Phospho-Amino Acid-Based Ionic Liquids: Formation of Zwitterionic Anions in the Presence of Acidic Side Chains. *Journal of Physical Chemistry B*, **2020**, 124, 1953-1964	3.4	7
47	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 = Mg(II)(H2O), Zn(II)). *Inorganic Chemistry*, **2011**, 50, 12116-25	5.1	7
46	Size-dependent solvation of p-H(2) in (4)He clusters: a quantum Monte Carlo analysis. *Journal of Chemical Physics*, **2009**, 130, 094906	3.9	7
45	Quenching efficiency of "hot" polar molecules by He buffer gas at ultralow energies: quantum results for MgH and LiH rotations. *European Physical Journal D*, **2008**, 48, 75-82	1.3	7
44	Recovery of nuclease produced by Lactococcus lactis using expanded bed ion exchange chromatography. *Biotechnology Letters*, **2006**, 28, 1033-9	3	7
43	CO Capture in Ionic Liquids Based on Amino Acid Anions With Protic Side Chains: a Computational Assessment of Kinetically Efficient Reaction Mechanisms. *ChemistryOpen*, **2020**, 9, 1153-1160	2.3	7
42	Reactive pathways toward parasitic release of singlet oxygen in metal-air batteries. *Npj Computational Materials*, **2021**, 7,	10.9	7

41	Naphthalenophane formaldehyde acetals as candidate structures for the generation of dynamic libraries via transacetalation processes. *Tetrahedron*, **2013**, 69, 2767-2774	2.4	6
40	Solvation of K+ in helium droplets. *European Physical Journal D*, **2007**, 43, 105-108	1.3	6
39	Solvent Structure around Lanthanoid(III) Ions in Liquid DMSO As Revealed by Polarizable Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2015**, 119, 13347-57	3.4	5
38	An experimental and theoretical investigation of XPS and NEXAFS of 5-halouracils. *Physical Chemistry Chemical Physics*, **2018**, 20, 6657-6667	3.6	5
37	Interaction anisotropy and quantum dynamics for vibrationally inelastic collisions of LiH(1Σ)with He(1S). *Chemical Physics*, **1998**, 237, 315-331	2.3	5
36	Ultra low-energy behavior of an ionic replacement reaction He3He+4+He4->He2+4+He3. *Physical Review A*, **2006**, 73,	2.6	5
35	CO Capture in Biocompatible Amino Acid Ionic Liquids: Exploring the Reaction Mechanisms for Bimolecular Absorption Processes. *Journal of Physical Chemistry B*, **2021**, 125, 5611-5619	3.4	5
34	Experimental and DFT/Time-Dependent DFT Studies on Neutral and One-Electron-Reduced Quinoxaline and Pyrazine Precursors and Their Mononuclear (PdII, PtII) Derivatives. *European Journal of Inorganic Chemistry*, **2014**, 2014, 3572-3581	2.3	4
33	Structural, energetic, and electronic properties of La(III)-dimethyl sulfoxide clusters. *Journal of Physical Chemistry A*, **2014**, 118, 11602-11	2.8	4
32	Collisional quenching at ultralow energies: controlling efficiency with internal state selection. *Journal of Chemical Physics*, **2007**, 127, 224303	3.9	4
31	Quenching of vibrationally excited molecules by ultracold collisions with ions: Controlling the scattering via changes of internal states. *Europhysics Letters*, **2007**, 77, 33001	1.6	4
30	Rotational cooling of molecular gases by positron impact at vanishing collision energies. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2005**, 38, 2069-2077	1.3	4
29	Photoexcitation of LiH2+ from selected initial states: A time-dependent model. *Journal of Chemical Physics*, **2002**, 117, 177-186	3.9	4
28	Testing Intermolecular Potentials with Scattering Experiments: He-CO Rotationally Inelastic Collisions. *Zeitschrift Fur Physikalische Chemie*, **2000**, 214,	3.1	4
27	Modelling biocompatible ionic liquids based on organic acids and amino acids: challenges for computational models and future perspectives. *Organic and Biomolecular Chemistry*, **2021**, 19, 4002-4013	3.9	4
26	Theoretical Insights into the Structure of the Aminotris(Methylenephosphonic Acid) (ATMP) Anion: A Possible Partner for Conducting Ionic Media. *Symmetry*, **2020**, 12, 920	2.7	3
25	Structure, Stability, and Electronic Properties of Dimethyl Sulfoxide and Dimethyl Formammide Clusters Containing Th(4.). *Journal of Physical Chemistry A*, **2016**, 120, 4778-88	2.8	3
24	Low and ultra-low energy chemical processes involving ions. *Physica Scripta*, **2009**, 80, 048117	2.6	3

23	A quantum modeling of the chemistry of LiH+ with He from ab initio calculations: Ionic reactions in He nanodroplets. *International Journal of Mass Spectrometry*, **2009**, 280, 57-64	1.9	3
22	Synthesis of new 2-phosphono-alpha-D-glycoside derivatives by stereoselective oxa-Michael addition to a D-galacto derived enone. *Carbohydrate Research*, **2008**, 343, 1133-41	2.9	3
21	Isotopic replacement in ionic systems: the 4He2+ + 3He-->3He 4He+ + 4He reaction. *Journal of Chemical Physics*, **2006**, 124, 044308	3.9	3
20	Strong intramolecular hydrogen bonding in protonated methylaminoalanine: A vibrational spectroscopic and computational study. *European Journal of Mass Spectrometry*, **2019**, 25, 133-141	1.1	3
19	On the formation of propylene oxide from propylene in space: gas-phase reactions. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	2
18	Solvation Properties of the Actinide Ion Th(IV) in DMSO and DMSO:Water Mixtures through Polarizable Molecular Dynamics. *Inorganic Chemistry*, **2017**, 56, 11929-11937	5.1	2
17	Raman Spectroscopy in Ionic Liquids Under Variable Thermodynamic and Environmental Conditions. *Soft and Biological Matter*, **2014**, 63-96	0.8	2
16	Theoretical Description of Ionic Liquids **2011**,		2
15	Theoretical treatment of the electronic excited states of the DMSO molecule: A challenge for current theoretical methods. *Chemical Physics*, **2010**, 377, 136-141	2.3	2
14	Ultralow-energy vibrational quenching in ionic collisions: Isotope effects in Li++D2 encounters. *Physical Review A*, **2008**, 77,	2.6	2
13	Perspectives in the Computational Modeling of New Generation, Biocompatible Ionic Liquids.. *Journal of Physical Chemistry B*, **2022**,	3.4	2
12	Experimental and Computational Investigation of Salophen-Zn Gas Phase Complexes with Cations: A Source of Possible Interference in Anionic Recognition. *Journal of Physical Chemistry A*, **2017**, 121, 7042-7050	2.8	1
11	Structural and energetic properties of La3+ in water/DMSO mixtures. *Journal of Molecular Structure* , **2017**, 1148, 381-387	3.4	1
10	QUANTUM STRUCTURING OF 4He ATOMS AROUND IONIC DOPANTS: ENERGETICS OF Li+, Na+ AND K+ FROM STOCHASTIC CALCULATIONS **2008**, 227-240		1
9	Reactions in non-aqueous alkali and alkaline-earth metal-oxygen batteries: a thermodynamic study. *Physical Chemistry Chemical Physics*, **2021**, 23, 24487-24496	3.6	1
8	Theoretical Description of Ionic Liquids. *Soft and Biological Matter*, **2014**, 127-148	0.8	1
7	Hydrogen bonding in biocompatible ionic liquids: an ab-initio characterization of dimeric interactions. *Electronic Structure*, **2021**, 3, 025004	2.6	1
6	Assessing the propensity toward ionization in nanosized clusters of protic ionic liquids by Ab-initio methods. *Chemical Physics*, **2022**, 552, 111365	2.3	0

5	Disclosing the hierarchical structure of ionic liquid mixtures by multiscale computational methods **2021**, 1-67		0
4	A Computational Analysis of the Reaction of SO2 with Amino Acid Anions: Implications for Its Chemisorption in Biobased Ionic Liquids. *Molecules*, **2022**, 27, 3604	4.8	0
3	Excited state dynamics of Zn-salophen complexes.. *Photochemical and Photobiological Sciences*, **2022**, 1	4.2	
2	Study of the Electronic Structure of Alkali Peroxides and Their Role in the Chemistry of Metal-Oxygen Batteries. *Journal of Physical Chemistry A*, **2021**, 125, 9368-9376	2.8	
1	Advanced Raman Spectroscopy Detection of Oxidative Damage in Nucleic Acid Bases: Probing Chemical Changes and Intermolecular Interactions in Guanosine at Ultralow Concentration. *Analytical Chemistry*, **2021**, 93, 10825-10833	7.8	