

Enrico Bodo

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Excited state dynamics of Zn-salophen complexes.. <i>Photochemical and Photobiological Sciences</i> , 2022 , 1	4.2	
147	Perspectives in the Computational Modeling of New Generation, Biocompatible Ionic Liquids.. <i>Journal of Physical Chemistry B</i> , 2022 ,	3.4	2
146	Assessing the propensity toward ionization in nanosized clusters of protic ionic liquids by Ab-initio methods. <i>Chemical Physics</i> , 2022 , 552, 111365	2.3	0
145	A Computational Analysis of the Reaction of SO ₂ with Amino Acid Anions: Implications for Its Chemisorption in Biobased Ionic Liquids. <i>Molecules</i> , 2022 , 27, 3604	4.8	0
144	Reactions in non-aqueous alkali and alkaline-earth metal-oxygen batteries: a thermodynamic study. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 24487-24496	3.6	1
143	Study of the Electronic Structure of Alkali Peroxides and Their Role in the Chemistry of Metal-Oxygen Batteries. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 9368-9376	2.8	
142	Assessing the Structure of Protic Ionic Liquids Based on Triethylammonium and Organic Acid Anions. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 2781-2792	3.4	8
141	CO Capture in Biocompatible Amino Acid Ionic Liquids: Exploring the Reaction Mechanisms for Bimolecular Absorption Processes. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 5611-5619	3.4	5
140	Hydrogen bonding in biocompatible ionic liquids: an ab-initio characterization of dimeric interactions. <i>Electronic Structure</i> , 2021 , 3, 025004	2.6	1
139	Advanced Raman Spectroscopy Detection of Oxidative Damage in Nucleic Acid Bases: Probing Chemical Changes and Intermolecular Interactions in Guanosine at Ultralow Concentration. <i>Analytical Chemistry</i> , 2021 , 93, 10825-10833	7.8	
138	Reactive pathways toward parasitic release of singlet oxygen in metal-air batteries. <i>Npj Computational Materials</i> , 2021 , 7,	10.9	7
137	Cholinium amino acid-based ionic liquids. <i>Biophysical Reviews</i> , 2021 , 13, 147-160	3.7	12
136	Disclosing the hierarchical structure of ionic liquid mixtures by multiscale computational methods 2021 , 1-67		0
135	Modelling biocompatible ionic liquids based on organic acids and amino acids: challenges for computational models and future perspectives. <i>Organic and Biomolecular Chemistry</i> , 2021 , 19, 4002-4013	3.9	4
134	Theoretical Insights into the Structure of the Aminotris(Methylenephosphonic Acid) (ATMP) Anion: A Possible Partner for Conducting Ionic Media. <i>Symmetry</i> , 2020 , 12, 920	2.7	3
133	Ab Initio Molecular Dynamics Study of Phospho-Amino Acid-Based Ionic Liquids: Formation of Zwitterionic Anions in the Presence of Acidic Side Chains. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 1953-1964	3.4	7
132	Structural Features of Triethylammonium Acetate through Molecular Dynamics. <i>Molecules</i> , 2020 , 25,	4.8	9

131	Superoxide Anion Disproportionation Induced by Li and H : Pathways to O Release in Li-O Batteries. <i>ChemPhysChem</i> , 2020 , 21, 2060-2067	3.2	11
130	CO Capture in Ionic Liquids Based on Amino Acid Anions With Protic Side Chains: a Computational Assessment of Kinetically Efficient Reaction Mechanisms. <i>ChemistryOpen</i> , 2020 , 9, 1153-1160	2.3	7
129	Ultra-Fast-VUV Photoemission Study of UV Excited 2-Nitrophenol. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 1295-1302	2.8	10
128	Structural Features of Cholinium Based Protic Ionic Liquids through Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 5568-5576	3.4	13
127	Vibrational signatures of curcumin's chelation in copper(II) complexes: An appraisal by IRMPD spectroscopy. <i>Journal of Chemical Physics</i> , 2019 , 150, 165101	3.9	7
126	On the formation of propylene oxide from propylene in space: gas-phase reactions. <i>Theoretical Chemistry Accounts</i> , 2019 , 138, 1	1.9	2
125	Strong intramolecular hydrogen bonding in protonated N-methylaminoalanine: A vibrational spectroscopic and computational study. <i>European Journal of Mass Spectrometry</i> , 2019 , 25, 133-141	1.1	3
124	Hydrogen Bonding Features in Cholinium-Based Protic Ionic Liquids from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 2635-2645	3.4	30
123	An experimental and theoretical investigation of XPS and NEXAFS of 5-halouracils. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 6657-6667	3.6	5
122	Isomerization patterns and proton transfer in ionic liquids constituents as probed by ab-initio computation. <i>Journal of Molecular Liquids</i> , 2018 , 249, 1075-1082	6	8
121	Hydrogen Bonding as a Clustering Agent in Protic Ionic Liquids: Like-Charge vs Opposite-Charge Dimer Formation. <i>ACS Omega</i> , 2018 , 3, 10589-10600	3.9	15
120	Unexpected proton mobility in the bulk phase of cholinium-based ionic liquids: new insights from theoretical calculations. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 11869-11880	3.6	27
119	Adenosine monophosphate recognition by zinc-salophen complexes: IRMPD spectroscopy and quantum modeling study. <i>Journal of Molecular Spectroscopy</i> , 2017 , 335, 108-116	1.3	11
118	Experimental and Computational Investigation of Salophen-Zn Gas Phase Complexes with Cations: A Source of Possible Interference in Anionic Recognition. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 7042-7050 ¹	3.8	1
117	Solvation Properties of the Actinide Ion Th(IV) in DMSO and DMSO:Water Mixtures through Polarizable Molecular Dynamics. <i>Inorganic Chemistry</i> , 2017 , 56, 11929-11937	5.1	2
116	Structural and energetic properties of La3+ in water/DMSO mixtures. <i>Journal of Molecular Structure</i> , 2017 , 1148, 381-387	3.4	1
115	Amino Acid Oxidation: A Combined Study of Cysteine Oxo Forms by IRMPD Spectroscopy and Simulations. <i>Chemistry - A European Journal</i> , 2016 , 22, 17239-17250	4.8	16
114	Structure, Stability, and Electronic Properties of Dimethyl Sulfoxide and Dimethyl Formamide Clusters Containing Th(4.). <i>Journal of Physical Chemistry A</i> , 2016 , 120, 4778-88	2.8	3

113	Theoretical study of ionic liquids based on the cholinium cation. Ab initio simulations of their condensed phases. <i>Journal of Chemical Physics</i> , 2016 , 144, 104504	3.9	30
112	Conformational Change in the Mechanism of Inclusion of Ketoprofen in β -Cyclodextrin: NMR Spectroscopy, Ab Initio Calculations, Molecular Dynamics Simulations, and Photoreactivity. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 10668-10678	3.4	14
111	Solvent Structure around Lanthanoid(III) Ions in Liquid DMSO As Revealed by Polarizable Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 13347-57	3.4	5
110	Interaction and dynamics of ionic liquids based on choline and amino acid anions. <i>Journal of Chemical Physics</i> , 2015 , 142, 234502	3.9	43
109	Lanthanum(III) and Lutetium(III) in Nitrate-Based Ionic Liquids: A Theoretical Study of Their Coordination Shell. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 11833-8	3.4	14
108	Interaction of a long alkyl chain protic ionic liquid and water. <i>Journal of Chemical Physics</i> , 2014 , 140, 204503	3.9	32
107	Silver nanoparticles linked by a Pt-containing organometallic dithiol bridge: study of local structure and interface by XAFS and SR-XPS. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 11719-28	3.6	25
106	Experimental and DFT/Time-Dependent DFT Studies on Neutral and One-Electron-Reduced Quinoxaline and Pyrazine Precursors and Their Mononuclear (PdII, PtII) Derivatives. <i>European Journal of Inorganic Chemistry</i> , 2014 , 2014, 3572-3581	2.3	4
105	Amino acid anions in organic ionic compounds. An ab initio study of selected ion pairs. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 2471-86	3.4	40
104	Structural, energetic, and electronic properties of La(III)-dimethyl sulfoxide clusters. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 11602-11	2.8	4
103	Anion recognition by uranyl-salophen derivatives as probed by infrared multiple photon dissociation spectroscopy and ab initio modeling. <i>Chemistry - A European Journal</i> , 2014 , 20, 11783-92	4.8	12
102	Raman Spectroscopy in Ionic Liquids Under Variable Thermodynamic and Environmental Conditions. <i>Soft and Biological Matter</i> , 2014 , 63-96	0.8	2
101	Theoretical Description of Ionic Liquids. <i>Soft and Biological Matter</i> , 2014 , 127-148	0.8	1
100	A prototypical ionic liquid explored by ab initio molecular dynamics and Raman spectroscopy. <i>Journal of Chemical Physics</i> , 2013 , 139, 144309	3.9	34
99	The soft X-ray absorption spectrum of the allyl free radical. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 1310-8	3.6	41
98	Probing the competition among different coordination motifs in metal-ciprofloxacin complexes through IRMPD spectroscopy and DFT calculations. <i>Inorganic Chemistry</i> , 2013 , 52, 103-12	5.1	9
97	Naphthalenophane formaldehyde acetals as candidate structures for the generation of dynamic libraries via transacetalation processes. <i>Tetrahedron</i> , 2013 , 69, 2767-2774	2.4	6
96	Conformational isomerisms and nano-aggregation in substituted alkylammonium nitrates ionic liquids: an x-ray and computational study of 2-methoxyethylammonium nitrate. <i>Journal of Chemical Physics</i> , 2013 , 138, 184506	3.9	27

95	Structural changes of conjugated Pt-containing polymetallaynes exposed to gamma ray radiation doses. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 8768-74	2.8	18
94	The interpretation of diffraction patterns of two prototypical protic ionic liquids: a challenging task for classical molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 13024-32	3.4	59
93	Unravelling the structure of protic ionic liquids with theoretical and experimental methods: ethyl-, propyl- and butylammonium nitrate explored by Raman spectroscopy and DFT calculations. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 13878-88	3.4	74
92	Infrared multiple photon dissociation spectroscopy of ciprofloxacin: Investigation of the protonation site. <i>Chemical Physics</i> , 2012 , 398, 124-128	2.3	15
91	Optical behavior of conjugated Pt-containing polymetallaynes exposed to gamma-ray radiation doses. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 8047-53	3.4	14
90	Structure of the molten salt methyl ammonium nitrate explored by experiments and theory. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 13149-61	3.4	49
89	Charge exchange in collisions of beryllium with its ion. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 19026-35	3.6	13
88	Structure of geminal imidazolium bis(trifluoromethylsulfonyl)imide dicationic ionic liquids: a theoretical study of the liquid phase. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 14341-7	3.4	35
87	Structural flexibility and role of vicinal 2-thienyl rings in 2,3-dicyano-5,6-di(2-thienyl)-1,4-pyrazine, [(CN) ₂ Th ₂ Pyz], its palladium(II) complex [(CN) ₂ Th ₂ Pyz(PdCl ₂) ₂], and the related pentametallic pyrazinoporphyrazines [(PdCl ₂) ₄ Th ₈ TPyzPz ₄ M] (M = Mg(II)(H ₂ O), Zn(II)). <i>Inorganic Chemistry</i> , 2011 , 50, 12116-25	5.1	7
86	Theoretical Description of Ionic Liquids 2011 ,		2
85	Photoinversion of sulfoxides as a source of diversity in dynamic combinatorial chemistry. <i>Organic Letters</i> , 2011 , 13, 142-5	6.2	18
84	X-Ray absorption spectroscopy investigation of 1-alkyl-3-methylimidazolium bromide salts. <i>Journal of Chemical Physics</i> , 2011 , 135, 074505	3.9	29
83	Structural Determination of Ionic Liquids with Theoretical Methods: C8mimBr and C8mimCl. Strength and Weakness of Current Force Fields. <i>Journal of Physical Chemistry Letters</i> , 2010 , 1, 1095-1100	6.4	31
82	The structure of geminal imidazolium bis(trifluoromethylsulfonyl)amide ionic liquids: a theoretical study of the gas phase ionic complexes. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 12506-12	2.8	22
81	Structural properties of 1-alkyl-3-methylimidazolium bis((trifluoromethyl)sulfonyl)amide ionic liquids: X-ray diffraction data and molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 16398-407	3.4	92
80	Theoretical treatment of the electronic excited states of the DMSO molecule: A challenge for current theoretical methods. <i>Chemical Physics</i> , 2010 , 377, 136-141	2.3	2
79	Near resonance charge exchange in ion-atom collisions of lithium isotopes. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 15085-91	2.8	22
78	Low and ultra-low energy chemical processes involving ions. <i>Physica Scripta</i> , 2009 , 80, 048117	2.6	3

77	Size-dependent solvation of p-H(2) in (4)He clusters: a quantum Monte Carlo analysis. <i>Journal of Chemical Physics</i> , 2009 , 130, 094906	3.9	7
76	Spin-driven structural effects in alkali doped (4)He clusters from quantum calculations. <i>Journal of Chemical Physics</i> , 2009 , 130, 224903	3.9	25
75	A quantum modeling of the chemistry of LiH ⁺ with He from ab initio calculations: Ionic reactions in He nanodroplets. <i>International Journal of Mass Spectrometry</i> , 2009 , 280, 57-64	1.9	3
74	Computing a three-dimensional electronic energy manifold for the LiH + H Li + H ₂ chemical reaction. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 1121-8	2.8	39
73	Anionic microsolvation in helium droplets: OH ⁻ (He) _N structures from classical and quantum calculations. <i>Journal of Chemical Physics</i> , 2008 , 128, 134511	3.9	20
72	Vibrational cooling of spin-stretched dimer states by He buffer gas: quantum calculations for Li ₂ (a 3Sigma(u ⁺)) at ultralow energies. <i>Journal of Chemical Physics</i> , 2008 , 128, 224312	3.9	13
71	Ultra-cold ion-atom collisions: near resonant charge exchange. <i>New Journal of Physics</i> , 2008 , 10, 033024	2.9	32
70	Nanoscopic phase changes in doped 4 He droplets. <i>Europhysics Letters</i> , 2008 , 82, 23001	1.6	19
69	Ultralow-energy vibrational quenching in ionic collisions: Isotope effects in Li ⁺⁺ D ₂ encounters. <i>Physical Review A</i> , 2008 , 77,	2.6	2
68	Chemical solutions in a quantum solvent: anionic electrolytes in 4He nanodroplets. <i>ChemPhysChem</i> , 2008 , 9, 1323-30	3.2	19
67	Energetics and structures of charged helium clusters: comparing stabilities of dimer and trimer cationic cores. <i>ChemPhysChem</i> , 2008 , 9, 2618-24	3.2	11
66	ASPIN: An all spin scattering code for atom-molecule rovibrationally inelastic cross sections. <i>Computer Physics Communications</i> , 2008 , 179, 821-838	4.2	36
65	Synthesis of new 2-phosphono-alpha-D-glycoside derivatives by stereoselective oxa-Michael addition to a D-galacto derived enone. <i>Carbohydrate Research</i> , 2008 , 343, 1133-41	2.9	3
64	Quenching efficiency of "hot" polar molecules by He buffer gas at ultralow energies: quantum results for MgH and LiH rotations. <i>European Physical Journal D</i> , 2008 , 48, 75-82	1.3	7
63	Ionic interactions and collision dynamics in cold traps: rotational quenching of OH(1 Σ^+) by Rb(2S). <i>European Physical Journal D</i> , 2008 , 49, 85-92	1.3	13
62	QUANTUM STRUCTURING OF 4He ATOMS AROUND IONIC DOPANTS: ENERGETICS OF Li ⁺ , Na ⁺ AND K ⁺ FROM STOCHASTIC CALCULATIONS 2008 , 227-240		1
61	Microsolvation of cationic dimers in 4He droplets: geometries of A ₂ (He) _N (A=Li, Na, K) from optimized energies. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 12289-94	2.8	20
60	Low energy H+CO scattering revisited. <i>Astronomy and Astrophysics</i> , 2007 , 475, L15-L18	5.1	29

59	Microsolvation of an ionic dopant in small (4)He clusters: OH ⁺ ((3) σ)((4)He)(N) via genetic algorithm optimizations. <i>ChemPhysChem</i> , 2007 , 8, 93-100	3.2	17
58	Solvation of K ⁺ in helium droplets. <i>European Physical Journal D</i> , 2007 , 43, 105-108	1.3	6
57	Quenching of molecular ions by He buffer loading at ultralow energies: rotational cooling of OH ⁺ (Σ) from quantum calculations. <i>European Physical Journal D</i> , 2007 , 44, 65-72	1.3	12
56	Rotational cooling efficiency upon molecular ionization: the case of Li ₂ ($a_3\Sigma^+$) and Li ₂ + (X $^2\Sigma^+$) interacting with 4He. <i>European Physical Journal D</i> , 2007 , 45, 267-272	1.3	10
55	Interaction of NH((X) ³ Σ^+)) with Rb and Cs atoms: similarities and differences from an highly correlated ab initio study. <i>Theoretical Chemistry Accounts</i> , 2007 , 117, 649-662	1.9	16
54	Bosonic helium clusters doped by alkali metal cations: interaction forces and analysis of their most stable structures. <i>Theoretical Chemistry Accounts</i> , 2007 , 118, 53-65	1.9	26
53	Production, formulation and antagonistic activity of the biocontrol like-yeast <i>Aureobasidium pullulans</i> against <i>Penicillium expansum</i> . <i>Biotechnology Letters</i> , 2007 , 29, 553-9	3	26
52	Bosonic helium droplets with cationic impurities: onset of electrostriction and snowball effects from quantum calculations. <i>Journal of Chemical Physics</i> , 2007 , 126, 124319	3.9	49
51	Collisional quenching at ultralow energies: controlling efficiency with internal state selection. <i>Journal of Chemical Physics</i> , 2007 , 127, 224303	3.9	4
50	Collisional quenching of rotations in lithium dimers by ultracold helium: the Li ₂ ($a_3\Sigma^+$) and Li ₂ + (X $^2\Sigma^+$) targets. <i>Journal of Chemical Physics</i> , 2007 , 127, 244315	3.9	8
49	Ionic dopants in He droplets: cluster energies from a variational and diffusion Monte Carlo approach. <i>Physica Scripta</i> , 2007 , 76, C104-C110	2.6	21
48	Sympathetic cooling of NH(X $^3\Sigma$) molecules by Rb and Cs atoms at ultralow energies. <i>Physical Review A</i> , 2007 , 75,	2.6	19
47	Collisions of NH(Σ) with Rb and Cs at ultralow energies: A quantum study of rotational cooling efficiency. <i>Physical Review A</i> , 2007 , 76,	2.6	11
46	Quenching of vibrationally excited molecules by ultracold collisions with ions: Controlling the scattering via changes of internal states. <i>Europhysics Letters</i> , 2007 , 77, 33001	1.6	4
45	OH(X $^1\Sigma$) collisions with 4He(1S) at vanishing energies: a quantum analysis of rotational quenching efficiency. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2006 , 39, S1203-S1213	1.3	13
44	Isotopic replacement in ionic systems: the 4He ²⁺ + 3He \rightarrow 3He 4He ⁺ + 4He reaction. <i>Journal of Chemical Physics</i> , 2006 , 124, 044308	3.9	3
43	Ultra low-energy behavior of an ionic replacement reaction He ³ He ⁴⁺ + He ⁴⁺ \rightarrow He ²⁺ + 4He ³ . <i>Physical Review A</i> , 2006 , 73,	2.6	5
42	Vibrational quenching at ultralow energies: Calculations of the Li ₂ ($\tilde{g}+1;\tilde{g}$) + He superelastic scattering cross sections. <i>Physical Review A</i> , 2006 , 73,	2.6	18

41	Quantum scattering of OH(X ¹ ₂) with He(S ₁): Propensity features in rotational relaxation at ultralow energies. <i>Physical Review A</i> , 2006 , 73,	2.6	23
40	Ionic dimers in He droplets: interaction potentials for Li ₂ (+)-He, Na ₂ (+)-He, and K ₂ (+)-He and stability of the smaller clusters. <i>Journal of Chemical Physics</i> , 2006 , 124, 74320	3.9	17
39	IONIC OH AS DOPANT OF HELIUM DROPLETS: AB INITIO POTENTIAL ENERGY SURFACES FOR OH+(3 ¹ ₁)-4He, OH-(1 ¹ ₁)-4He, AND STABLE STRUCTURES OF THEIR SMALLER CLUSTERS. <i>Journal of Theoretical and Computational Chemistry</i> , 2006 , 05, 543-564	1.8	15
38	Microsolvation of Li ⁺ in bosonic helium clusters. I. Many-body effects on the structures of the small aggregates. <i>Computational Materials Science</i> , 2006 , 35, 261-267	3.2	21
37	Collisional quenching of molecular ro-vibrational energy by He buffer loading at ultralow energies. <i>International Reviews in Physical Chemistry</i> , 2006 , 25, 313-351	7	43
36	Adaptive clustering of a quantum solvent: the LiH ⁺ cation in bosonic helium from stochastic calculations. <i>European Physical Journal D</i> , 2006 , 40, 377-385	1.3	12
35	Recovery of nuclease produced by <i>Lactococcus lactis</i> using expanded bed ion exchange chromatography. <i>Biotechnology Letters</i> , 2006 , 28, 1033-9	3	7
34	Ionic reactions in He nanodroplets: the [LiHHe] ⁺ complex and its possible energy pathways into products from ab initio calculations. <i>Journal of Chemical Physics</i> , 2005 , 122, 224312	3.9	10
33	Microsolvation of Li(+) in Small He Clusters. Li(+)Hen Species from Classical and Quantum Calculations. <i>Journal of Chemical Theory and Computation</i> , 2005 , 1, 1045-54	6.4	31
32	Microsolvation of LiH ⁺ in helium clusters: many-body effects and additivity models for the interaction forces. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 4252-60	2.8	12
31	Energetics and structure of the bound states in a lithium complex: The (LiH ₂) ⁺ electronic ground state. <i>Chemical Physics</i> , 2005 , 314, 135-142	2.3	30
30	The Weak Li ₂ He Interaction Revisited: a Combined Ab-initio and Empirical Modelling.. <i>Journal of Low Temperature Physics</i> , 2005 , 138, 259-264	1.3	22
29	Rotational cooling of molecular gases by positron impact at vanishing collision energies. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2005 , 38, 2069-2077	1.3	4
28	Neutral and ionic dopants in helium clusters: interaction forces for the and complexes. <i>Molecular Physics</i> , 2005 , 103, 3223-3231	1.7	11
27	Chemical reactions in the limit of zero kinetic energy: virtual states and Ramsauer minima in F + H ₂ HF + H. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2004 , 37, 3641-3648	1.3	71
26	Ab initio quantum dynamics with very weak van der Waals interactions: Structure and stability of small Li ₂ (1 ¹ _g σ ⁺)-(He) _n clusters. <i>Journal of Chemical Physics</i> , 2004 , 120, 9160-6	3.9	21
25	Rotationally inelastic collisions of electrons with (H ₂) and (N ₂) molecules: converged space-frame calculations at low energies. <i>European Physical Journal D</i> , 2004 , 29, 357-365	1.3	14
24	Charged cores in ionized (He ₄) clusters III: A quantum modeling for the collisional relaxation dynamics. <i>European Physical Journal D</i> , 2004 , 30, 363-368	1.3	18

23	Features of chemical reactions at vanishing kinetic energy: the presence of internally hot reagents. <i>European Physical Journal D</i> , 2004 , 31, 423-427	1.3	17
22	Rotational cooling of Li ₂ (1 Σ^+_g) molecules by ultracold collisions with a helium gas buffer. <i>Theoretical Chemistry Accounts</i> , 2004 , 112, 263	1.9	12
21	A modified Variable-Phase algorithm for multichannel scattering with long-range potentials. <i>Computer Physics Communications</i> , 2003 , 151, 187-198	4.2	52
20	Three-dimensional reactive surfaces for the LiH ₂ ⁺ system: an analysis of accurate ab initio results. <i>Chemical Physics</i> , 2003 , 287, 335-348	2.3	36
19	The gas-phase lithium chemistry in the early universe: elementary processes, interaction forces and quantum dynamics. <i>Physics Reports</i> , 2003 , 384, 85-119	27.7	66
18	Collisional Cooling of Polar Diatomics in 3He and 4He Buffer Gas: A Quantum Calculation at Ultralow Energies. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 7328-7336	2.8	12
17	Accurate potential energy surfaces for the study of lithium-hydrogen ionic reactions. <i>Journal of Chemical Physics</i> , 2003 , 119, 11241-11248	3.9	61
16	Rotational and Vibrational Excitation of CO Molecules by Collisions with 4He Atoms. <i>Astrophysical Journal</i> , 2002 , 571, 1015-1020	4.7	44
15	Quenching of vibrationally excited CO(Σ^2) molecules by ultra-cold collisions with 4He atoms. <i>Chemical Physics Letters</i> , 2002 , 353, 127-130	2.5	20
14	F+D ₂ reaction at ultracold temperatures. <i>Journal of Chemical Physics</i> , 2002 , 116, 9222-9227	3.9	94
13	Rotational quenching in ionic systems at ultracold temperatures. <i>Physical Review Letters</i> , 2002 , 89, 2832-2834	2.1	23
12	Photoexcitation of LiH ₂ ⁺ from selected initial states: A time-dependent model. <i>Journal of Chemical Physics</i> , 2002 , 117, 177-186	3.9	4
11	The reaction of F + D ₂ at ultra-low temperatures: the effect of rotational excitation. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2002 , 35, 2391-2396	1.3	25
10	Computed orientational anisotropy and vibrational couplings for the LiH + H interaction potential. <i>European Physical Journal D</i> , 2001 , 15, 321-329	1.3	14
9	Possible reaction paths in the LiH ₂ ⁺ chemistry: a computational analysis of the interaction forces. <i>Chemical Physics</i> , 2001 , 271, 309-321	2.3	42
8	A multireference valence bond approach to electronic excited states. <i>Journal of Chemical Physics</i> , 2001 , 115, 2917-2925	3.9	28
7	Reactive Behavior of the [LiH ₂] ⁺ System II. Collision-Induced Dissociation and Collinear Reaction Dynamics of LiH ₂ ⁺⁺ +H from Quantum Time Dependent Calculations. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 10994-11000	2.8	27
6	Reactive Behavior of the [LiH ₂] ⁺ System I. Evaluation of the Lower-lying Electronic Potentials for the Collinear Geometries. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 10986-10993	2.8	30

5	Testing Intermolecular Potentials with Scattering Experiments: He-CO Rotationally Inelastic Collisions. <i>Zeitschrift Fur Physikalische Chemie</i> , 2000 , 214,	3.1	4
4	Testing van der Waals interactions with quantum dynamics: Repulsive anisotropy and well depth in the LiH+He system. <i>Journal of Chemical Physics</i> , 2000 , 113, 11071-11078	3.9	13
3	Spatial Energetics of Protonated LiH: Lower-Lying Potential Energy Surfaces from Valence Bond Calculations. <i>Journal of Physical Chemistry A</i> , 2000 , 104, 11972-11982	2.8	30
2	Interaction anisotropy and quantum dynamics for vibrationally inelastic collisions of LiH(1 σ) with He(1S). <i>Chemical Physics</i> , 1998 , 237, 315-331	2.3	5
1	Vibrational Heating Efficiency of LiH Molecules in Collision with He Atoms \square <i>Journal of Physical Chemistry A</i> , 1998 , 102, 9390-9398	2.8	17