Manuel Alcami

List of Publications by Year
in descending order

187	5,079	94433	118850
papers	citations	37 h-index	62 g-index

194	194	194	5216
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Mechanical Isolation of Highly Stable Antimonene under Ambient Conditions. Advanced Materials, 2016, 28, 6332-6336.	21.0	444
2	Charge-transfer-induced structural rearrangements at both sides of organic/metal interfaces. Nature Chemistry, 2010, 2, 374-379.	13.6	273
3	Computational chemistry: A useful (sometimes mandatory) tool in mass spectrometry studies. Mass Spectrometry Reviews, 2001, 20, 195-245.	5.4	160
4	Long-range magnetic order in a purely organic 2D layer adsorbed on epitaxial graphene. Nature Physics, 2013, 9, 368-374.	16.7	158
5	Role of Dispersion Forces in the Structure of Graphene Monolayers on Ru Surfaces. Physical Review Letters, 2011, 106, 186102.	7.8	129
6	Cu+ binding energies. Dramatic failure of the G2 method vs. good performance of the B3LYP approach. Chemical Physics Letters, 2000, 320, 129-138.	2.6	93
7	Atomically resolved phase transition of fullerene cations solvated in helium droplets. Nature Communications, 2016, 7, 13550.	12.8	84
8	Theoretical study of ionization potentials and dissociation energies of Cnq+ fullerenes (n=50â€“60,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	3.0	78
9	Modeling the Interactions between Peptide Functions and Cu(I): Formamideâ^'Cu+ Reactions in the Gas Phase. Journal of the American Chemical Society, 1998, 120, 5411-5426.	13.7	75
10	Dynamics of Glycine Dications in the Gas Phase: Ultrafast Intramolecular Hydrogen Migration versus Coulomb Repulsion. Journal of Physical Chemistry Letters, 2013, 4, 3903-3909.	4.6	74
11	Crossover Siteâ€Selectivity in the Adsorption of the Fullerene Derivative PCBM on Au(111). Angewandte Chemie - International Edition, 2007, 46, 7874-7877.	13.8	70
12	Gas-Phase Deprotonation of Uracilâ^'Cu2+ and Thiouracilâ^'Cu2+ Complexes. Journal of Physical Chemistry A, 2006, 110, 1943-1950.	2.5	69
13	Bond activation by protonation in the gas phase. Chemical Physics Letters, 1990, 172, 471-477.	2.6	68
14	Structures, Energetics, and Dynamics of Helium Adsorbed on Isolated Fullerene Ions. Physical Review Letters, 2012, 108, 076101.	7.8	68
15	Are the Thiouracils Sulfur Bases in the Gas-phase?. Journal of Physical Chemistry A, 2000, 104, 5122-5130.	2.5	66
16	Association of Cu2+with Uracil and Its Thio Derivatives: A Theoretical Study. ChemPhysChem, 2004, 5, 1871-1878.	2.1	66
17	Unimolecular Reactivity of Uracilâ€“Cu2+ Complexes in the Gas Phase. ChemPhysChem, 2007, 8, 181-187.	2.1	64
18	Ultrafast Nonadiabatic Fragmentation Dynamics of Doubly Charged Uracil in a Gas Phase. Physical Review Letters, 2011, 107, 023202.	7.8	63

#	Article	IF	Citations
19	Molecular Growth Inside of Polycyclic Aromatic Hydrocarbon Clusters Induced by Ion Collisions. Journal of Physical Chemistry Letters, 2015, 6, 1536-1542.	4.6	62
20	Formations of Dumbbell<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">C</mml:mi><mml:mn>118</mml:mn></mml:msub></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">C</mml:mi><mml:mn>119</mml:mn></mml:msub></mml:math>inside Clusters of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:m	7.8	61
21	Modeling intrinsic basicities and acidities. Journal of Physical Organic Chemistry, 2002, 15, 174-186.	1.9	57
22	Fullerene C50: Sphericity takes over, not strain. Chemical Physics Letters, 2005, 407, 153-158.	2.6	56
23	G2ab initio calculations on three-membered rings: Role of hydrogen atoms. Journal of Computational Chemistry, 1998, 19, 1072-1086.	3.3	55
24	Coulomb Stability Limit of Highly ChargedC60q+Fullerenes. Physical Review Letters, 2005, 95, 013401.	7.8	55
25	The performance of density-functional theory in challenging cases: Halogen oxides. Journal of Chemical Physics, 2000, 112, 6131-6140.	3.0	49
26	A molecular orbital study of azole-lithium(1+) complexes. The Journal of Physical Chemistry, 1989, 93, 3929-3936.	2.9	47
27	Gas-Phase Reactivity of Uracil, 2-Thiouracil, 4-Thiouracil, and 2,4-Dithiouracil towards the Cu+ Cation: A DFT Study. ChemPhysChem, 2003, 4, 1011-1016.	2.1	45
28	Fragmentation of Highly Excited Small Neutral Carbon Clusters. Physical Review Letters, 2004, 93, 063401.	7.8	45
29	Adsorption of Hydrogen Molecules on Carbon Nanotubes Using Quantum Chemistry and Molecular Dynamics. Journal of Physical Chemistry A, 2016, 120, 6451-6458.	2.5	45
30	A Multicoincidence Study of Fragmentation Dynamics in Collision of Î³â€Aminobutyric Acid with Lowâ€Energy Ions. Chemistry - A European Journal, 2012, 18, 9321-9332.	3.3	44
31	Structure and Electronic Properties of Fullerenes C52q+: Is C522+an Exception to the Pentagon Adjacency Penalty Rule?. ChemPhysChem, 2005, 6, 92-100.	2.1	43
32	Surfaceâ€Supported Robust 2D Lanthanideâ€Carboxylate Coordination Networks. Small, 2015, 11, 6358-6364.	10.0	43
33	Structure and electronic properties of highly charged C60 and C58 fullerenes. Journal of Chemical Physics, 2005, 123, 184306.	3.0	41
34	Cage connectivity and frontier Ï€ orbitals govern the relative stability of charged fullerene isomers. Nature Chemistry, 2015, 7, 927-934.	13.6	41
35	Experimental and theoretical study of lithium(1+) affinities of methyldiazoles. The Journal of Physical Chemistry, 1990, 94, 4796-4804.	2.9	39
36	Stable Nonâ€IPR C₆₀ and C₇₀ Fullerenes Containing a Uniform Distribution of Pyrenes and Adjacent Pentagons. ChemPhysChem, 2008, 9, 861-866.	2.1	39

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37	Determination of Energy-Transfer Distributions in Ionizing Ion-Molecule Collisions. Physical Review Letters, 2016, 117, 073201.	7.8	39
38	Role of Cu+Association on the Formamide â†' Formamidic Acid â†' (Aminohydroxy)carbene Isomerizations in the Gas Phase. Journal of Physical Chemistry A, 1998, 102, 4652-4659.	2.5	38
39	Enhanced Li+ binding energies of some azines: a molecular orbital study. Theoretica Chimica Acta, 1990, 77, 1-15.	0.8	36
40	Internal energy dependence in x-ray-induced molecular fragmentation: An experimental and theoretical study of thiophene. Physical Review A, 2015, 91, .	2.5	36
41	Key Structural Motifs To Predict the Cage Topology in Endohedral Metallofullerenes. Journal of the American Chemical Society, 2016, 138, 1551-1560.	13.7	36
42	Relative Stability of Empty Exohedral Fullerenes: Ï€ Delocalization versus Strain and Steric Hindrance. Journal of the American Chemical Society, 2017, 139, 1609-1617.	13.7	36
43	Nitrogen inversion barriers in three-membered rings. Anab initiomolecular orbital study. Journal of Computational Chemistry, 1989, 10, 468-478.	3.3	35
44	Lattice-matched versus lattice-mismatched models to describe epitaxial monolayer graphene on Ru(0001). Physical Review B, 2013, 88, .	3.2	35
45	Elastic Response of Graphene Nanodomes. ACS Nano, 2013, 7, 2927-2934.	14.6	35
46	Stabilization of nitrogen-containing three-membered rings by proton and lithium ion association in the gas phase. Journal of the American Chemical Society, 1993, 115, 11074-11083.	13.7	34
47	Statistical fragmentation of small neutral carbon clusters. Physical Review A, 2005, 71, .	2.5	34
48	Electron localization in epitaxial graphene on Ru(0001) determined by moirÃ© corrugation. Physical Review B, 2012, 85, .	3.2	34
49	Ultrafast Damage Following Radiationâ€Induced Oxidation of Uracil in Aqueous Solution. Angewandte Chemie - International Edition, 2013, 52, 3160-3163.	13.8	34
50	Non-statistical fragmentation of PAHs and fullerenes in collisions with atoms. International Journal of Mass Spectrometry, 2014, 365-366, 260-265.	1.5	34
51	Roadmap on dynamics of molecules and clusters in the gas phase. European Physical Journal D, 2021, 75, 1.	1.3	32
52	Structure, Dissociation Energies, and Harmonic Frequencies of Small Doubly Charged Carbon Clusters Cn2+(n= 3â^'9)â€. Journal of Physical Chemistry A, 2002, 106, 10782-10789.	2.5	31
53	Absolute Charge Transfer and Fragmentation Cross Sections inHe2+â^'C60Collisions. Physical Review Letters, 2008, 100, 183401.	7.8	31
54	Theoretical investigation of the ultrafast dissociation of ionised biomolecules immersed in water: Direct and indirect effects. Mutation Research - Reviews in Mutation Research, 2010, 704, 45-53.	5.5	31

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55	Multiple ionization and hydrogen loss from neutral and positively-charged coronene. Journal of Chemical Physics, 2014, 140, 204307.	3.0	31
56	First- and second-electron affinities ofC60andC70isomers. Physical Review A, 2007, 76, .	2.5	30
57	A density functional theory study of the manganese-phthalocyanine. Theoretical Chemistry Accounts, 2011, 128, 497-503.	1.4	30
58	Ionization potentials and dissociation energies of neutral, singly and doubly charged Cn fullerenes from n=20 to 70. International Journal of Mass Spectrometry, 2006, 252, 133-141.	1.5	29
59	Unusual hydroxyl migration in the fragmentation of Î²-alanine dication in the gas phase. Physical Chemistry Chemical Physics, 2015, 17, 16767-16778.	2.8	29
60	Experimental and Theoretical Investigation of the Reactions between Glucose and Cu+ in the Gas Phase. Journal of Physical Chemistry A, 2002, 106, 2641-2651.	2.5	28
61	Magic and hot giant fullerenes formed inside ion irradiated weakly bound C60 clusters. Journal of Chemical Physics, 2010, 133, 104301.	3.0	28
62	Enhanced aluminum(1+) binding energies of some azoles: a theoretical study of azole-X+ (X = Na, K, Al) complexes. The Journal of Physical Chemistry, 1992, 96, 3022-3029.	2.9	27
63	Formation dynamics of fullerene dimers<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msubsup><mml:mi>C</mml:mi><mml:mrow><mml:mn>118</mml:mn><mml:mn>119</mml:mn></mml:mrow></mml:msubsup></mml:math> and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msubsup><mml:mi>C</mml:mi><mml:mrow><mml:mn>120</mml:mn></mml:mrow></mml:msubsup></mml:math>. Physical Review A, 2014, 89, .	2.5	27
64	Structural Patterns in Fullerenes Showing Adjacent Pentagons: C20 to C72. Journal of Nanoscience and Nanotechnology, 2007, 7, 1329-1338.	0.9	26
65	Cu+ reactivity trends in sp, sp2, and sp3 nitrogen, phosphorus, and arsenic containing bases. International Journal of Mass Spectrometry, 2000, 201, 215-231.	1.5	25
66	Unimolecular Reactivity of Strong Metalâ€“Cation Complexes in the Gas Phase: Ethylenediamineâ€“Cu+. Chemistry - A European Journal, 2004, 10, 2927-2934.	3.3	24
67	Theoretical study of the structure of self-assembled monolayers of short alkylthiolates on Au(111) and Ag(111): the role of induced substrate reconstruction and chainâ€“chain interactions. Physical Chemistry Chemical Physics, 2011, 13, 9353.	2.8	24
68	Probing the Site-Dependent Kondo Response of Nanostructured Graphene with Organic Molecules. Nano Letters, 2014, 14, 4560-4567.	9.1	24
69	Chain-Length and Temperature Dependence of Self-Assembled Monolayers of Alkylthiolates on Au(111) and Ag(111) Surfaces. Journal of Physical Chemistry A, 2014, 118, 4138-4146.	2.5	23
70	Antimonene: Mechanical Isolation of Highly Stable Antimonene under Ambient Conditions (Adv. Mater.) Tj ETQq0 0 0 rgBT /Overlock 10	21.0	23
71	Exploring the Potential Energy Surface of the Association of Cu+to Oxaziridine, Nitrosomethane, and Formaldoxime. Journal of Physical Chemistry A, 1998, 102, 10120-10127.	2.5	22
72	Basicity of some carbonyl compounds towards iodine monochloride: experimental and theoretical study. New Journal of Chemistry, 2001, 25, 509-517.	2.8	22

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73	Theoretical Survey of the Potential Energy Surface of Ethylenediamine + Cu+Reactions. Journal of Physical Chemistry A, 2004, 108, 8367-8372.	2.5	22
74	Size dependence of ionization potentials and dissociation energies for neutral and singly-charged Cn fullerenes (n=40â€“70). Chemical Physics Letters, 2005, 416, 14-17.	2.6	22
75	Ionization and fragmentation of water clusters by fast highly charged ions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2009, 42, 075101.	1.5	22
76	Fragmentation Dynamics of Doubly Charged Methionine in the Gas Phase. Journal of Physical Chemistry A, 2014, 118, 1374-1383.	2.5	22
77	Understanding the self-assembly of TCNQ on Cu(111): a combined study based on scanning tunnelling microscopy experiments and density functional theory simulations. RSC Advances, 2016, 6, 15071-15079.	3.6	22
78	Polypeptide formation in clusters of Î²-alanine amino acids by single ion impact. Nature Communications, 2020, 11, 3818.	12.8	22
79	Fragmentation of small neutral carbon clusters. International Journal of Mass Spectrometry, 2006, 252, 126-132.	1.5	21
80	Understanding the Supramolecular Selfâ€Assembly of the Fullerene Derivative PCBM on Gold Surfaces. ChemPhysChem, 2008, 9, 1030-1035.	2.1	21
81	Ions colliding with clusters of fullerenesâ€”Decay pathways and covalent bond formations. Journal of Chemical Physics, 2013, 139, 034309.	3.0	21
82	Quantum chemistry in environmental pesticide risk assessment. Pest Management Science, 2017, 73, 2199-2202.	3.4	21
83	Topology-Based Approach to Predict Relative Stabilities of Charged and Functionalized Fullerenes. Journal of Chemical Theory and Computation, 2018, 14, 1791-1810.	5.3	21
84	Modelling Intrinsic Basicities: The Use of the Electrostatic Potentials and the Atoms-in-Molecules Theory. Theoretical and Computational Chemistry, 1996, 3, 407-456.	0.4	20
85	Ionization potentials, dissociation energies and statistical fragmentation of neutral and positively charged small carbon clusters. Brazilian Journal of Physics, 2006, 36, 529-533.	1.4	20
86	Adsorption of Benzene on Cu(100) and on Cu(100) Covered with an Ultrathin NaCl Film: Moleculeâ€“Substrate Interaction and Decoupling. Journal of Physical Chemistry C, 2015, 119, 4062-4071.	3.1	20
87	Structure, Ionization, and Fragmentation of Neutral and Positively Charged Hydrogenated Carbon Clusters: C_nH_m^{q+} (n = 1â€“5, m =) Tj ETQq1 1 0.784314 rgB		
88	M₃C: A Computational Approach To Describe Statistical Fragmentation of Excited Molecules and Clusters. Journal of Chemical Theory and Computation, 2017, 13, 992-1009.	5.3	20
89	Ab Initio Molecular Orbital Study of XO2+ (X = F, Cl, Br, I) Systems. Journal of Physical Chemistry A, 1999, 103, 2793-2800.	2.5	19
90	The Final Steps of the Oppolzer Cyclization: Mechanism of the Insertion of Alkenes into Allylpalladium(II) Complexes. Chemistry - A European Journal, 2003, 9, 96-105.	3.3	19

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91	Controlling the spatial arrangement of organic magnetic anions adsorbed on epitaxial graphene on Ru(0001). Nanoscale, 2014, 6, 15271-15279.	5.6	19
92	Furan Fragmentation in the Gas Phase: New Insights from Statistical and Molecular Dynamics Calculations. Journal of Physical Chemistry A, 2018, 122, 4153-4166.	2.5	19
93	Gas-Phase Basicity of 2,7-Dimethyl-[1,2,4]-Triazepine Thio Derivatives. Journal of Physical Chemistry A, 2002, 106, 7383-7389.	2.5	18
94	Understanding Sulfone Behavior in Palladium-Catalyzed Domino Reactions with Aryl Iodides. Chemistry - A European Journal, 2006, 12, 4576-4583.	3.3	18
95	Bonding in exohedral metalâ€“fullerene cationic complexes. RSC Advances, 2014, 4, 53010-53020.	3.6	18
96	Study of the interaction between short alkanethiols from ab initio calculations. Physical Chemistry Chemical Physics, 2010, 12, 7555.	2.8	17
97	AB initioMO study of the halogen cation basicities of some organic bases. Journal of Physical Organic Chemistry, 1991, 4, 177-191.	1.9	16
98	A theoretical study of the interaction between Ni+ and small oxygen- and nitrogen-containing bases. International Journal of Mass Spectrometry, 2002, 217, 119-129.	1.5	16
99	Theoretical study of the stability of multiply charged C70 fullerenes. Journal of Chemical Physics, 2007, 127, 104308.	3.0	16
100	Growth and Structure of Self-assembled Monolayers of a TTF Derivative on Au(111). Journal of Physical Chemistry C, 2010, 114, 6503-6510.	3.1	16
101	Ordered arrays of metalâ€“organic magnets at surfaces. Journal of Physics Condensed Matter, 2013, 25, 484007.	1.8	16
102	Charge transfer-assisted self-limited decyanation reaction of TCNQ-type electron acceptors on Cu(100). Chemical Communications, 2014, 50, 833-835.	4.1	16
103	Stability of the glycine cation in the gas phase after interaction with multiply charged ions. European Physical Journal D, 2014, 68, 1.	1.3	16
104	An AB initio molecular orbital study of the structure, energetics and bond activation of Al+ complexes. Computational and Theoretical Chemistry, 1991, 234, 357-371.	1.5	14
105	Optimization of extended basis sets and assessment of different theoretical schemes for Pb containing compounds. Chemical Physics Letters, 2004, 383, 561-565.	2.6	14
106	Density functional theory study of multiply ionized weakly bound fullerene dimers. Journal of Chemical Physics, 2009, 130, 224302.	3.0	14
107	Prototropic tautomerism of 3,5-(oxo/thioxo) derivatives of 2,7-dimethyl-1,2,4-triazepinesElectronic supplementary information (ESI) available: the B3LYP/6-31G* optimized geometries of all the structures included in Fig. 1 and the corresponding TS. See http://www.rsc.org/suppdata/nj/b1/b109397e/. New Journal of Chemistry, 2002, 26, 711-719.	2.8	13
108	Why Does Pivalaldehyde (Trimethylacetaldehyde) Unexpectedly Seem More Basic Than 1-Adamantanecarbaldehyde in the Gas Phase? FT-ICR and High-Level Ab Initio Studies. Chemistry - A European Journal, 2005, 11, 1826-1832.	3.3	13

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109	Production of doubly-charged highly reactive species from the long-chain amino acid GABA initiated by Ar⁹⁺ionization. Physical Chemistry Chemical Physics, 2017, 19, 19609-19618.	2.8	13
110	Is C50 a superaromat? Evidence from electronic structure and ring current calculations. Physical Chemistry Chemical Physics, 2016, 18, 11653-11660.	2.8	12
111	Ab initio molecular orbital treatment of hydroxylamine-X+-water and hydroxylamine-X+-ammonia (X =) Tj ETQq1 1 0.784314 rgBT /Ov	1.9	11
112	Experimental and theoretical study of C2H4OAl+ complexes in the gas phase. The Journal of Physical Chemistry, 1992, 96, 8309-8317.	2.9	11
113	Stability of multiply charged fullerene anions and cations. Physical Review A, 2009, 80, .	2.5	11
114	Commensurate Solidâ€“Solid Phase Transitions in Self-Assembled Monolayers of Alkylthiolates Lying on Metal Surfaces. Journal of the American Chemical Society, 2012, 134, 13224-13227.	13.7	11
115	Density functional theory study of the structure and vibrational modes of acrylonitrile adsorbed on Cu(100). Physical Chemistry Chemical Physics, 2013, 15, 1288-1295.	2.8	11
116	Tuning Intermolecular Charge Transfer in Donorâ€“Acceptor Two-Dimensional Crystals on Metal Surfaces. Journal of Physical Chemistry C, 2017, 121, 23505-23510.	3.1	11
117	Study of polarization effects in three-membered-ring heterocycles. Computational and Theoretical Chemistry, 1988, 165, 99-114.	1.5	10
118	Gas-Phase Chemistry of Ethyl and Vinyl Amines, Phosphines, and Arsines:â€‰ A DFT Study of the Structure and Stability of Their Cu+ Complexes. Journal of Physical Chemistry A, 2002, 106, 9306-9312.	2.5	10
119	Triaziridine and tetrazetidine vs. cyclic water trimer and tetramer: A computational approach to the relationship between molecular and supramolecular conformational analysis. Physical Chemistry Chemical Physics, 2002, 4, 2123-2129.	2.8	10
120	Simple bond patterns predict the stability of Dielsâ€“Alder adducts of empty fullerenes. Chemical Communications, 2018, 54, 4156-4159.	4.1	10
121	Synthesis, X-ray Structure, and Properties of 2-(1â€˜-Pyridin-2â€˜-one)Benzimidazole. Journal of Physical Chemistry B, 2001, 105, 12759-12770.	2.6	9
122	Generalized structural motif model for studying the thermodynamic stability of fullerenes: from C₆₀to graphene passing through giant fullerenes. Physical Chemistry Chemical Physics, 2017, 19, 19646-19655.	2.8	9
123	A general approach to study molecular fragmentation and energy redistribution after an ionizing event. Physical Chemistry Chemical Physics, 2021, 23, 1859-1867.	2.8	9
124	Fragmentation of neutral Cn clusters (n ? 9): experimental and theoretical investigations. European Physical Journal D, 2003, 24, 149-152.	1.3	8
125	Surface assembly of porphyrin nanorods with one-dimensional zincâ€“oxygen spinal cords. CrystEngComm, 2011, 13, 5591.	2.6	8
126	Multiple electron capture, excitation, and fragmentation in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">C</mml:mi><mml:mrow><mml:msup><mml:mrow /><mml:mrow><mml:mn>6</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup><mml:mo>â^’</mml:mo></mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>collisions. Physical Review A, 2014, 90, .	2.5	8

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127	Pesticide byproducts formation: Theoretical study of the protonation of alloxydim degradation products. Computational and Theoretical Chemistry, 2018, 1143, 9-19.	2.5	8
128	Potential energy surfaces of C2v and D3h ozone complexes with Li+. Journal of Chemical Physics, 1995, 103, 253-265.	3.0	7
129	Exohedral interaction in cationic lithium metallofullerenes. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	7
130	Ultrafast nonadiabatic fragmentation dynamics of biomolecules. Journal of Physics: Conference Series, 2014, 488, 012037.	0.4	7
131	Theoretical study of the interaction between molecular hydrogen and [MC₆₀]⁺ complexes. RSC Advances, 2016, 6, 27447-27451.	3.6	7
132	Computational Study of the Structure and Degradation Products of Alloxydim Herbicide. Journal of Physical Chemistry A, 2018, 122, 3909-3918.	2.5	7
133	Aromaticity, Coulomb repulsion, Ï€ delocalization or strain: who is who in endohedral metallofullerene stability?. Physical Chemistry Chemical Physics, 2019, 21, 124-131.	2.8	7
134	Hydrogenated polycyclic aromatic hydrocarbons: isomerism and aromaticity. Physical Chemistry Chemical Physics, 2020, 22, 21968-21976.	2.8	7
135	Structure of <mml:math altimg="si1.gif" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://www.elsevier.com/x	3.0	6
136	Formation of Self-Assembled Chains of Tetrathiafulvalene on a Cu(100) Surface. Journal of Physical Chemistry A, 2011, 115, 13080-13087.	2.5	6
137	The role of spin-forbidden processes in N+(3P) + NH3 reactions in the gas phase. Physical Chemistry Chemical Physics, 2001, 3, 179-183.	2.8	5
138	Gas-Phase Chemistry of Ethynylamine, -Phosphine and -Arsine. Structure and Stability of their Cu+ and Ni+ Complexes. ChemPhysChem, 2003, 4, 72-78.	2.1	5
139	Unraveling the Factors That Control Soft Landing of Small Silyl Ions on Fluorinated Self-Assembled Monolayers. Journal of Physical Chemistry C, 2014, 118, 10159-10169.	3.1	5
140	<i>N</i>-Acetylglycine Cation Tautomerization Enabled by the Peptide Bond. Journal of Physical Chemistry A, 2015, 119, 9581-9589.	2.5	5
141	When is the Bellâ€“Evansâ€“Polanyi principle fulfilled in Dielsâ€“Alder reactions of fullerenes?. Physical Chemistry Chemical Physics, 2020, 22, 8846-8852.	2.8	5
142	Hydrogenation of C₂₄ Carbon Clusters: Structural Diversity and Energetic Properties. Journal of Physical Chemistry A, 2021, 125, 5273-5288.	2.5	5
143	Isomers of Hydrogenated Polycyclic Aromatic Hydrocarbons Explain the Presence of Infrared Bands in the 3 Î¼m Region. Astrophysical Journal, 2020, 899, 18.	4.5	5
144	Thermochemistry of the reactions between CN+ and H2O in the gas phase. Molecular Physics, 2001, 99, 1129-1137.	1.7	4

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145	Perturbation of the intramolecular hydrogen bonds of glucose by Cu+association. International Journal of Quantum Chemistry, 2002, 86, 138-144.	2.0	4
146	Structure and reactivity of C54q+(q= 0, 1, 2 and 4) fullerenes. Physical Chemistry Chemical Physics, 2005, 7, 3756.	2.8	4
147	Time-dependent density functional theory molecular dynamics simulation of doubly charged uracil in gas phase. Open Physics, 2014, 12, .	1.7	4
148	Thermal Transition from a Disordered, 2D Network to a Regular, 1D, Fe(II)â€“DCNQI Coordination Network. Journal of Physical Chemistry C, 2016, 120, 16712-16721.	3.1	4
149	Fully versus constrained statistical fragmentation of carbon clusters and their heteronuclear derivatives. Journal of Chemical Physics, 2019, 150, 144301.	3.0	4
150	Thermochemistry of the Reactions F+(3P,1D) + PH3in the Gas Phase. Journal of Physical Chemistry A, 2000, 104, 8075-8080.	2.5	3
151	Computational Studies on the Cyclization of Polycyclic Aromatic Hydrocarbons in the Synthesis of Curved Aromatic Derivatives. ChemPhysChem, 2006, 7, 475-481.	2.1	3
152	Charge-Transfer-Induced Isomerization of DCNQI on Cu(100). Journal of Physical Chemistry C, 2014, 118, 27388-27392.	3.1	3
153	Fragmentation network of doubly charged methionine: Interpretation using graph theory. Journal of Chemical Physics, 2016, 145, 094302.	3.0	3
154	Controlling the diversity of ion-induced fragmentation pathways by N-methylation of amino acids. Physical Chemistry Chemical Physics, 2022, 24, 941-954.	2.8	3
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