Peter Politzer

List of Publications by Year
in descending order

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		3515	3638
356	35,826	90	180
papers	citations	h-index	g-index

369	369	369	11933
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Halogen bonding: the Ïƒ-hole. Journal of Molecular Modeling, 2007, 13, 291-296.	0.8	2,004
2	Definition of the halogen bond (IUPAC Recommendations 2013). Pure and Applied Chemistry, 2013, 85, 1711-1713.	0.9	1,554
3	Halogen bonding and other Ïƒ-hole interactions: a perspective. Physical Chemistry Chemical Physics, 2013, 15, 11178.	1.3	1,401
4	Halogen bonding: an electrostatically-driven highly directional noncovalent interaction. Physical Chemistry Chemical Physics, 2010, 12, 7748.	1.3	1,389
5	An overview of halogen bonding. Journal of Molecular Modeling, 2007, 13, 305-311.	0.8	1,284
6	The electrostatic potential: an overview. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 153-163.	6.2	1,049
7	Quantitative analysis of molecular surfaces: areas, volumes, electrostatic potentials and average local ionization energies. Journal of Molecular Modeling, 2010, 16, 1679-1691.	0.8	985
8	The fundamental nature and role of the electrostatic potential in atoms and molecules. Theoretical Chemistry Accounts, 2002, 108, 134-142.	0.5	965
9	Expansion of the Ïƒ-hole concept. Journal of Molecular Modeling, 2009, 15, 723-729.	0.8	669
10	Halogen Bonding: An Interim Discussion. ChemPhysChem, 2013, 14, 278-294.	1.0	620
11	Ïƒ-Holes, Ï€-holes and electrostatically-driven interactions. Journal of Molecular Modeling, 2012, 18, 541-548.	0.8	545
12	Ïƒ-hole bonding: molecules containing group VI atoms. Journal of Molecular Modeling, 2007, 13, 1033-1038.	0.8	475
13	Use of the electrostatic potential at the molecular surface to interpret and predict nucleophilic processes. The Journal of Physical Chemistry, 1990, 94, 3959-3961.	2.9	377
14	Halogen bond tunability I: the effects of aromatic fluorine substitution on the strengths of halogen-bonding interactions involving chlorine, bromine, and iodine. Journal of Molecular Modeling, 2011, 17, 3309-3318.	0.8	374
15	Surface electrostatic potentials of halogenated methanes as indicators of directional intermolecular interactions. International Journal of Quantum Chemistry, 1992, 44, 57-64.	1.0	370
16	Ïƒ-hole bonding between like atoms; a fallacy of atomic charges. Journal of Molecular Modeling, 2008, 14, 659-665.	0.8	368
17	An electrostatic interaction correction for improved crystal density prediction. Molecular Physics, 2009, 107, 2095-2101.	0.8	365
18	Average local ionization energies on the molecular surfaces of aromatic systems as guides to chemical reactivity. Canadian Journal of Chemistry, 1990, 68, 1440-1443.	0.6	363

#	Article	IF	Citations
19	Halogen bonding and the design of new materials: organic bromides, chlorides and perhaps even fluorides as donors. Journal of Molecular Modeling, 2007, 13, 643-650.	0.8	342
20	A predicted new type of directional noncovalent interaction. International Journal of Quantum Chemistry, 2007, 107, 2286-2292.	1.0	341
21	Perspectives on halogen bonding and other Ïƒ-hole interactions: Lex parsimoniae (Occamâ€™s Razor). Computational and Theoretical Chemistry, 2012, 998, 2-8.	1.1	333
22	Average local ionization energy: A review. Journal of Molecular Modeling, 2010, 16, 1731-1742.	0.8	328
23	The Ïƒ-hole revisited. Physical Chemistry Chemical Physics, 2017, 19, 32166-32178.	1.3	319
24	Ïƒ-Hole bonding and hydrogen bonding: Competitive interactions. International Journal of Quantum Chemistry, 2007, 107, 3046-3052.	1.0	305
25	BrÂ·Â·Â·O Complexes as Probes of Factors Affecting Halogen Bonding: Interactions of Bromobenzenes and Bromopyrimidines with Acetone. Journal of Chemical Theory and Computation, 2009, 5, 155-163.	2.3	303
26	Links between surface electrostatic potentials of energetic molecules, impact sensitivities and Câ€“NO₂/Nâ€“NO₂bond dissociation energies. Molecular Physics, 2009, 107, 89-97.	0.8	280
27	Statistical analysis of the molecular surface electrostatic potential: an approach to describing noncovalent interactions in condensed phases. Computational and Theoretical Chemistry, 1998, 425, 107-114.	1.5	255
28	A possible crystal volume factor in the impact sensitivities of some energetic compounds. Journal of Molecular Modeling, 2010, 16, 895-901.	0.8	250
29	Directional tendencies of halogen and hydrogen bonds. International Journal of Quantum Chemistry, 2010, 110, 2823-2832.	1.0	243
30	A comparative analysis of Hartree-Fock and Kohn-Sham orbital energies. Theoretical Chemistry Accounts, 1998, 99, 83-87.	0.5	237
31	Directional Weak Intermolecular Interactions: Ïƒ-Hole Bonding. Australian Journal of Chemistry, 2010, 63, 1598.	0.5	235
32	Mathematical modeling and physical reality in noncovalent interactions. Journal of Molecular Modeling, 2015, 21, 52.	0.8	234
33	Blue shifts vs red shifts in Ïƒ-hole bonding. Journal of Molecular Modeling, 2008, 14, 699-704.	0.8	231
34	Molecular electrostatic potentials and noncovalent interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1326.	6.2	231
35	Fluorine-Centered Halogen Bonding: A Factor in Recognition Phenomena and Reactivity. Crystal Growth and Design, 2011, 11, 4238-4246.	1.4	225
36	Calculation of heats of sublimation and solid phase heats of formation. Molecular Physics, 1997, 91, 923-928.	0.8	222

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37	Trends in Ïƒ-hole strengths and interactions of F3MX molecules (M = C, Si, Ge and X = F, Cl, Br, I). Journal of Molecular Modeling, 2013, 19, 2739-2746.	0.8	219
38	Molecular surface electrostatic potentials in relation to noncovalent interactions in biological systems. International Journal of Quantum Chemistry, 2001, 85, 676-684.	1.0	217
39	The fluorine atom as a halogen bond donor, viz. a positive site. CrystEngComm, 2011, 13, 6593.	1.3	217
40	Polarizability and volume. Journal of Chemical Physics, 1993, 98, 4305-4306.	1.2	216
41	A relationship between the charge capacity and the hardness of neutral atoms and groups. Journal of Chemical Physics, 1987, 86, 1072-1073.	1.2	203
42	Relationships between dissociation energies and electrostatic potentials of Cî—¸NO2 bonds: applications to impact sensitivities. Journal of Molecular Structure, 1996, 376, 419-424.	1.8	190
43	Halogen bond tunability II: the varying roles of electrostatic and dispersion contributions to attraction in halogen bonds. Journal of Molecular Modeling, 2013, 19, 4651-4659.	0.8	190
44	High Performance, Low Sensitivity: Conflicting or Compatible?. Propellants, Explosives, Pyrotechnics, 2016, 41, 414-425.	1.0	189
45	Effects of amino and nitro substituents upon the electrostatic potential of an aromatic ring. Journal of the American Chemical Society, 1984, 106, 855-860.	6.6	183
46	Statistically-based interaction indices derived from molecular surface electrostatic potentials: a general interaction properties function (GIPF). Computational and Theoretical Chemistry, 1994, 307, 55-64.	1.5	183
47	A misconception concerning the electronic density distribution of an atom. Theoretica Chimica Acta, 1975, 38, 159-163.	0.9	182
48	Simultaneous Ïƒâ€hole and hydrogen bonding by sulfurâ€•and seleniumâ€containing heterocycles. International Journal of Quantum Chemistry, 2008, 108, 2770-2781.	1.0	172
49	The complementary roles of molecular surface electrostatic potentials and average local ionization energies with respect to electrophilic processes. International Journal of Quantum Chemistry, 2002, 88, 19-27.	1.0	166
50	Properties of atoms in molecules. I. Proposed definition of the charge on an atom in a molecule. Journal of the American Chemical Society, 1970, 92, 6451-6454.	6.6	164
51	Family-independent relationships between computed molecular surface quantities and solute hydrogen bond acidity/basicity and solute-induced methanol Oâ€“H infrared frequency shifts. Canadian Journal of Chemistry, 1995, 73, 483-488.	0.6	164
52	Why are dimethyl sulfoxide and dimethyl sulfone such good solvents?. Journal of Molecular Modeling, 2008, 14, 689-697.	0.8	159
53	Comparison of Quantum Chemical Parameters and Hammett Constants in Correlating pKaValues of Substituted Anilines. Journal of Organic Chemistry, 2001, 66, 6919-6925.	1.7	158
54	Relationships between impact sensitivities and molecular surface electrostatic potentials of nitroaromatic and nitroheterocyclic molecules. Molecular Physics, 1995, 85, 1-8.	0.8	157

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55	Molecular Electrostatic Potentials and Chemical Reactivity. Reviews in Computational Chemistry, 2007, , 273-312.	1.5	153
56	Comparison of density functional and Hartree-Fock average local ionization energies on molecular surfaces. International Journal of Quantum Chemistry, 1998, 69, 607-613.	1.0	152
57	Some relations between electronic distribution and electronegativity. Journal of Chemical Physics, 1979, 71, 4218-4220.	1.2	151
58	Effects of strongly electron-attracting components on molecular surface electrostatic potentials: application to predicting impact sensitivities of energetic molecules. Molecular Physics, 1998, 93, 187-194.	0.8	151
59	Ïƒ-Hole Interactions of Covalently-Bonded Nitrogen, Phosphorus and Arsenic: A Survey of Crystal Structures. Crystals, 2014, 4, 12-31.	1.0	149
60	Molecular surface electrostatic potentials and local ionization energies of Group V-VII hydrides and their anions: Relationships for aqueous and gas-phase acidities. International Journal of Quantum Chemistry, 1993, 48, 73-88.	1.0	146
61	Ïƒ-Hole Interactions: Perspectives and Misconceptions. Crystals, 2017, 7, 212.	1.0	145
62	A perspective on quantum mechanics and chemical concepts in describing noncovalent interactions. Physical Chemistry Chemical Physics, 2018, 20, 30076-30082.	1.3	135
63	Correlations between the solvent hydrogen-bond-donating parameter .alpha. and the calculated molecular surface electrostatic potential. Journal of Organic Chemistry, 1991, 56, 6715-6717.	1.7	133
64	Ïƒ-Hole Bonding: A Physical Interpretation. Topics in Current Chemistry, 2014, 358, 19-42.	4.0	133
65	Sensitivity and the available free space per molecule in the unit cell. Journal of Molecular Modeling, 2011, 17, 2569-2574.	0.8	127
66	Ïƒâ€holes and Ï€â€holes: Similarities and differences. Journal of Computational Chemistry, 2018, 39, 464-471.	1.5	127
67	Average local ionization energies computed on the surfaces of some strained molecules. International Journal of Quantum Chemistry, 1990, 38, 645-653.	1.0	126
68	Reactivities of Sites on (5,5) Single-Walled Carbon Nanotubes with and without a Stone-Wales Defect. Journal of Chemical Theory and Computation, 2010, 6, 1351-1357.	2.3	126
69	Characteristic features of the electrostatic potentials of singly negative monoatomic ions. Journal of Chemical Physics, 1989, 90, 4370-4372.	1.2	125
70	Some new energy formulas for atoms and molecules. Journal of Chemical Physics, 1974, 61, 4258-4262.	1.2	124
71	Characterization of Surface Electrostatic Potentials of some (5,5) and (n,1) Carbon and Boron/Nitrogen Model Nanotubes. Nano Letters, 2003, 3, 21-28.	4.5	124
72	Some molecular/crystalline factors that affect the sensitivities of energetic materials: molecular surface electrostatic potentials, lattice free space and maximum heat of detonation per unit volume. Journal of Molecular Modeling, 2015, 21, 25.	0.8	124

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73	Correlations between the solvent hydrogen bond acceptor parameter .beta. and the calculated molecular electrostatic potential. Journal of Organic Chemistry, 1991, 56, 3734-3737.	1.7	122
74	The reaction force: Three key points along an intrinsic reaction coordinate. Journal of Chemical Sciences, 2005, 117, 467-472.	0.7	122
75	Polarization-induced Ïƒ-holes and hydrogen bonding. Journal of Molecular Modeling, 2012, 18, 2461-2469.	0.8	121
76	Impact sensitivity and crystal lattice compressibility/free space. Journal of Molecular Modeling, 2014, 20, 2223.	0.8	121
77	Computational prediction of standard gas, liquid, and solid-phase heats of formation and heats of vaporization and sublimation. International Journal of Quantum Chemistry, 2005, 105, 341-347.	1.0	119
78	Quantitative determination of the total local polarity (charge separation) in molecules. Molecular Physics, 1992, 76, 609-617.	0.8	118
79	Relationships between atomic chemical potentials, electrostatic potentials, and covalent radii. Journal of Chemical Physics, 1983, 79, 3859-3861.	1.2	114
80	Correlations between molecular electrostatic potentials and some experimentally-based indices of reactivity. Computational and Theoretical Chemistry, 1992, 256, 29-45.	1.5	114
81	Some approximate energy relationships for molecules. Journal of Chemical Physics, 1976, 64, 4239-4240.	1.2	107
82	Computational investigation of the structures and relative stabilities of amino/nitro derivatives of ethylene. Computational and Theoretical Chemistry, 1998, 452, 75-83.	1.5	107
83	Impact sensitivity and the maximum heat of detonation. Journal of Molecular Modeling, 2015, 21, 262.	0.8	107
84	Halogen bonding and beyond: factors influencing the nature of CNâ€“R and SiNâ€“R complexes with Fâ€“Cl and Cl2. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	102
85	The reaction force and the transition region of a reaction. Journal of Molecular Modeling, 2009, 15, 707-710.	0.8	101
86	Separation of core and valence regions in atoms. Journal of Chemical Physics, 1976, 64, 4634-4637.	1.2	99
87	Correct electrostatic treatment of noncovalent interactions: the importance of polarization. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 169-177.	6.2	97
88	Shock-sensitivity relationships for nitramines and nitroaliphatics. Chemical Physics Letters, 1991, 181, 78-82.	1.2	96
89	A computational analysis of the bonding in boron trifluoride and boron trichloride and their complexes with ammonia. Inorganic Chemistry, 1993, 32, 2622-2625.	1.9	94
90	An Overview of Strengths and Directionalities of Noncovalent Interactions: Ïƒ-Holes and Ï€-Holes. Crystals, 2019, 9, 165.	1.0	94

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91	Computational characterization of energetic materials. Computational and Theoretical Chemistry, 2001, 573, 1-10.	1.5	93
92	Electronegativity and the concept of charge capacity. Computational and Theoretical Chemistry, 1992, 259, 99-120.	1.5	91
93	Computational prediction of condensed phase properties from statistical characterization of molecular surface electrostatic potentials. Fluid Phase Equilibria, 2001, 185, 129-137.	1.4	89
94	Radial behavior of the average local ionization energies of atoms. Journal of Chemical Physics, 1991, 95, 6699-6704.	1.2	88
95	Relationships of molecular surface electrostatic potentials to some macroscopic properties. Chemical Physics, 1996, 204, 289-299.	0.9	85
96	Intuitive and counterintuitive noncovalent interactions of aromatic Ï€ regions with the hydrogen and the nitrogen of HCN. Journal of Computational Science, 2015, 10, 209-216.	1.5	83
97	Atomic polarizability, volume and ionization energy. Journal of Chemical Physics, 2002, 117, 8197-8202.	1.2	82
98	Relationships of critical constants and boiling points to computed molecular surface properties. The Journal of Physical Chemistry, 1993, 97, 9369-9373.	2.9	81
99	Reaction force constant and projected force constants of vibrational modes along the path of an intramolecular proton transfer reaction. Chemical Physics Letters, 2008, 456, 135-140.	1.2	80
100	Halogen bonding in hypervalent iodine and bromine derivatives: halonium salts. IUCrJ, 2017, 4, 411-419.	1.0	80
101	Electrostatic potentials of amine nitrogens as a measure of the total electron-attracting tendencies of substituents. Chemical Physics Letters, 1988, 152, 364-370.	1.2	79
102	C-NO2dissociation energies and surface electrostatic potential maxima in relation to the impact sensitivities of some nitroheterocyclic molecules. Molecular Physics, 1995, 86, 251-255.	0.8	79
103	Analysis of two intramolecular proton transfer processes in terms of the reaction force. Journal of Chemical Physics, 2004, 121, 4570-4576.	1.2	78
104	Electrostatics and Polarization in Ïƒâ€•and Ï€â€Hole Noncovalent Interactions: An Overview. ChemPhysChem, 2020, 21, 579-588.	1.0	78
105	Factors affecting the strengths of Ïƒ-hole electrostatic potentials. Journal of Computational Science, 2014, 5, 590-596.	1.5	76
106	The aromatic Cî—¸NO2 bond as a site for nucleophilic attack. Chemical Physics Letters, 1984, 111, 75-78.	1.2	75
107	An electrostatic correction for improved crystal density predictions of energetic ionic compounds. Molecular Physics, 2010, 108, 1391-1396.	0.8	75
108	Relationships between the aqueous acidities of some carbon, oxygen, and nitrogen acids and the calculated surface local ionization energies of their conjugate bases. Journal of Organic Chemistry, 1991, 56, 5012-5015.	1.7	74

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109	Quantitative Analyses of Molecular Surface Electrostatic Potentials in Relation to Hydrogen Bonding and Co-Crystallization. Crystal Growth and Design, 2015, 15, 3767-3774.	1.4	74
110	Proposed procedure for using electrostatic potentials to predict and interpret nucleophilic processes. The Journal of Physical Chemistry, 1982, 86, 4767-4771.	2.9	72
111	A computational study of the structures and electrostatic potentials of some azines and nitroazines. Computational and Theoretical Chemistry, 1989, 187, 95-108.	1.5	72
112	Reaction Force Decomposition of Activation Barriers To Elucidate Solvent Effects. Journal of Physical Chemistry A, 2007, 111, 2455-2457.	1.1	71
113	Detonation Performance and Sensitivity. Advances in Quantum Chemistry, 2014, 69, 1-30.	0.4	70
114	Electrostatic potentialâ€“electronic density relationships in atoms. Journal of Chemical Physics, 1980, 72, 3027-3033.	1.2	69
115	Octanol/water partition coefficients expressed in terms of solute molecular surface areas and electrostatic potentials. Journal of Organic Chemistry, 1993, 58, 7070-7073.	1.7	69
116	A relationship between experimentally determined pKas and molecular surface ionization energies for some azines and azoles. Journal of Organic Chemistry, 1991, 56, 2934-2936.	1.7	68
117	Comparative analysis of the electrostatic potentials of dibenzofuran and some dibenzo-p-dioxins. Journal of the American Chemical Society, 1986, 108, 915-918.	6.6	66
118	Calculated electrostatic potentials and local surface ionization energies of para-substituted anilines as measures of substituent effects. Canadian Journal of Chemistry, 1992, 70, 2209-2214.	0.6	66
119	Role of Polarization in Halogen Bonds. Australian Journal of Chemistry, 2014, 67, 451.	0.5	66
120	Chlorotrinitromethane and its exceptionally short carbonâ€“chlorine bond. Nature Chemistry, 2009, 1, 229-235.	6.6	65
121	Prediction of Aqueous Solvation Free Energies from Properties of Solute Molecular Surface Electrostatic Potentials. Journal of Physical Chemistry A, 1999, 103, 1853-1856.	1.1	64
122	Directional Noncovalent Interactions: Repulsion and Dispersion. Journal of Chemical Theory and Computation, 2013, 9, 2264-2275.	2.3	64
123	Investigation of relationships between solute molecule surface electrostatic potentials and solubilities in supercritical fluids. The Journal of Physical Chemistry, 1992, 96, 7938-7943.	2.9	62
124	Applications of calculated local surface ionization energies to chemical reactivity. Computational and Theoretical Chemistry, 1992, 255, 271-281.	1.5	62
125	Density functional study of dimers of dimethylnitramine. International Journal of Quantum Chemistry, 2000, 80, 184-192.	1.0	62
126	Molecular surface electrostatic potentials and anesthetic activity. Journal of Molecular Modeling, 2007, 13, 313-318.	0.8	62

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127	Complementarity of reaction force and electron localization function analyses of asynchronicity in bond formation in Dielsâ€“Alder reactions. Physical Chemistry Chemical Physics, 2014, 16, 6726.	1.3	62
128	Comparative analysis of electrostatic potential maxima and minima on molecular surfaces, as determined by three methods and a variety of basis sets. Journal of Computational Science, 2016, 17, 273-284.	1.5	62
129	Close contacts and noncovalent interactions in crystals. Faraday Discussions, 2017, 203, 113-130.	1.6	62
130	Nonlocal density functional calculation of gas phase heats of formation. Journal of Computational Chemistry, 1995, 16, 654-658.	1.5	59
131	Analysis of the Reaction Force for a Gas Phase SN2 Process:Â CH3Cl + H2O â†’ CH3OH + HClâ€. Journal of Physical Chemistry A, 2006, 110, 756-761.	1.1	59
132	Interaction and Polarization Energy Relationships in Ïƒ-Hole and Ï€-Hole Bonding. Crystals, 2020, 10, 76.	1.0	58
133	Comparative analysis of surface electrostatic potentials of carbon, boron/nitrogen and carbon/boron/nitrogen model nanotubes. Journal of Molecular Modeling, 2005, 11, 1-7.	0.8	57
134	A density functional/molecular dynamics study of the structure of liquid nitromethane. Journal of Chemical Physics, 1995, 102, 8281-8282.	1.2	56
135	Energetics of Aluminum Combustion. Journal of Physical Chemistry A, 2001, 105, 7473-7480.	1.1	56
136	Average Local Ionization Energies as a Route to Intrinsic Atomic Electronegativities. Journal of Chemical Theory and Computation, 2011, 7, 377-384.	2.3	55
137	Bond-order-bond-energy correlations. Chemical Physics Letters, 1986, 124, 527-530.	1.2	54
138	Hydrogenation and Fluorination of Graphene Models: Analysis via the Average Local Ionization Energy. Journal of Physical Chemistry A, 2012, 116, 8644-8652.	1.1	54
139	The reaction force constant: an indicator of the synchronicity in double proton transfer reactions. Physical Chemistry Chemical Physics, 2012, 14, 11125.	1.3	54
140	The reaction force constant as an indicator of synchronicity/nonsynchronicity in [4+2] cycloaddition processes. Physical Chemistry Chemical Physics, 2013, 15, 7311.	1.3	53
141	Fluorination promotes chalcogen bonding in crystalline solids. CrystEngComm, 2017, 19, 4955-4959.	1.3	53
142	A proposed interpretation of the destabilizing effect of hydroxyl groups on nitroaromatic molecules. Chemical Physics Letters, 1989, 158, 463-469.	1.2	52
143	Anomalous energy effects associated with the presence of aza nitrogens and nitro substituents in some strained systems. Computational and Theoretical Chemistry, 1990, 207, 193-200.	1.5	51
144	Computational characterization of nucleotide bases: Molecular surface electrostatic potentials and local ionization energies, and local polarization energies. International Journal of Quantum Chemistry, 2001, 83, 245-254.	1.0	50

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145	Electrostatic potentials on the molecular surfaces of cyclic ureides. The Journal of Physical Chemistry, 1991, 95, 844-848.	2.9	49
146	Computational study of the structure of dinitraminic acid, HN(NO2)2, and the energetics of some possible decomposition steps. Chemical Physics Letters, 1993, 216, 348-352.	1.2	48
147	Relationships between solute molecular properties and solubility in supercritical carbon dioxide. The Journal of Physical Chemistry, 1993, 97, 729-732.	2.9	48
148	Relationships between Lattice Energies and Surface Electrostatic Potentials and Areas of Anions. Journal of Physical Chemistry A, 1998, 102, 1018-1020.	1.1	47
149	Electrostatic potentials of some dibenzo-p-dioxins in relation to their biological activities. Theoretica Chimica Acta, 1987, 72, 507-517.	0.9	46
150	Reaction Force and Its Link to Diabatic Analysis: A Unifying Approach to Analyzing Chemical Reactions. Journal of Physical Chemistry Letters, 2010, 1, 2858-2862.	2.1	46
151	Perspectives on the reaction force constant. Journal of Molecular Modeling, 2013, 19, 4111-4118.	0.8	45
152	Observations on the Significance of the Electrostatic Potentials at the Nuclei of Atoms and Molecules. Israel Journal of Chemistry, 1980, 19, 224-232.	1.0	44
153	Density Functional Tight-Binding Studies of Carbon Nanotube Structures. Structural Chemistry, 2003, 14, 431-443.	1.0	44
154	Energy changes associated with some decomposition steps of 1,3,3-trinitroazetidine. A non-local density functional study. Chemical Physics Letters, 1993, 207, 27-30.	1.2	43
155	Local ionization energy and local polarizability. International Journal of Quantum Chemistry, 2004, 96, 394-401.	1.0	43
156	Electrostatically driven complexes of SiF₄ with amines. International Journal of Quantum Chemistry, 2009, 109, 3773-3780.	1.0	43
157	Electronegativityâ€”a perspective. Journal of Molecular Modeling, 2018, 24, 214.	0.8	43
158	Enthalpy and entropy factors in gas phase halogen bonding: compensation and competition. CrystEngComm, 2013, 15, 3145.	1.3	42
159	The Ïƒâ€Hole Coulombic Interpretation of Trihalide Anion Formation. ChemPhysChem, 2018, 19, 3044-3049.	1.0	42
160	The Hellmann-Feynman theorem: a perspective. Journal of Molecular Modeling, 2018, 24, 266.	0.8	42
161	The use and misuse of van der Waals radii. Structural Chemistry, 2021, 32, 623-629.	1.0	42
162	Hydrogen Bonding: A Coulombic Ïƒ-Hole Interaction. Journal of the Indian Institute of Science, 2020, 100, 21-30.	0.9	41

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163	The ï€-hole revisited. Physical Chemistry Chemical Physics, 2021, 23, 16458-16468.	1.3	41
164	Identifying the most energetic electrons in a molecule: The highest occupied molecular orbital and the average local ionization energy. Computational and Theoretical Chemistry, 2021, 1199, 113192.	1.1	41
165	Properties of atoms in molecules. Theoretica Chimica Acta, 1971, 23, 203-207.	0.9	40
166	Energetics of ammonium dinitramide decomposition steps. Computational and Theoretical Chemistry, 1998, 427, 123-129.	1.5	39
167	Variation of parameters in Becke-3 hybrid exchange-correlation functional. Journal of Computational Chemistry, 2000, 21, 227-238.	1.5	39
168	Relationships between computed molecular properties and solute-solvent interactions in supercritical solutions. The Journal of Physical Chemistry, 1993, 97, 5144-5148.	2.9	38
169	Molecular Dynamics Simulations of Energetic Solids. Structural Chemistry, 2002, 13, 105-113.	1.0	38
170	Bond Orders of Homonuclear Diatomic Molecules. Journal of Chemical Physics, 1969, 50, 2780-2781.	1.2	37
171	The use of the electrostatic potential at the molecular surface in recognition interactions: Dibenzo-p-dioxinsand related systems. Journal of Molecular Graphics, 1990, 8, 81-85.	1.7	37
172	Energetics of ammonium perchlorate decomposition steps. Computational and Theoretical Chemistry, 1998, 454, 229-235.	1.5	37
173	The unique role of the nitro group in intramolecular interactions: chloronitromethanes. Structural Chemistry, 2010, 21, 139-146.	1.0	37
174	Computational analysis of relative stabilities of polyazine N-oxides. Structural Chemistry, 2013, 24, 1965-1974.	1.0	37
175	Representation of C60 Solubilities in Terms of Computed Molecular Surface Electrostatic Potentials and Areas. The Journal of Physical Chemistry, 1995, 99, 12081-12083.	2.9	36
176	Perspectives on the Reaction Force. Advances in Quantum Chemistry, 2012, 64, 189-209.	0.4	36
177	Fine structure in the transition region: reaction force analyses of water-assisted proton transfers. Journal of Molecular Modeling, 2013, 19, 2689-2697.	0.8	36
178	Gaussian-2 and density functional studies of H2N?NO2 dissociation, inversion, and isomerization. International Journal of Quantum Chemistry, 1992, 44, 497-504.	1.0	35
179	Molecular Dynamics Simulations of Liquid Nitromethane. Journal of Physical Chemistry B, 1999, 103, 9738-9742.	1.2	35
180	Chapter 8 The average local ionization energy: concepts and applications. Theoretical and Computational Chemistry, 2007, 19, 119-137.	0.2	35

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181	Electrostatic potentials and covalent radii. Journal of Computational Chemistry, 2003, 24, 505-511.	1.5	34
182	Connection between the average local ionization energy and the Fukui function. Chemical Physics Letters, 2005, 407, 143-146.	1.2	34
183	Approximate radii for singly negative ions of 3d, 4d, and 5d metal atoms. Journal of Chemical Physics, 1989, 91, 5123-5124.	1.2	33
184	Anomalous energy effects in some aliphatic and alicyclic aza systems and their nitro derivatives. The Journal of Physical Chemistry, 1990, 94, 2320-2323.	2.9	33
185	A computational analysis of the structural features and reactive behavior of some heterocyclic aromatic N-oxides. Computational and Theoretical Chemistry, 1991, 236, 283-296.	1.5	33
186	Can Counterâ€Intuitive Halogen Bonding Be Coulombic?. ChemPhysChem, 2021, 22, 1201-1207.	1.0	33
187	Density functional study of the structure and some decomposition reactions of the dinitramide anion N(NO2)2â^'. Computational and Theoretical Chemistry, 1993, 287, 235-240.	1.5	32
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