Shridhar R Gadre

List of Publications by Year
in descending order

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214 papers	8,529 citations	34105 52 h-index	58581 82 g-index
215 all docs	215 docs citations	215 times ranked	3957 citing authors

#	Article	IF	Citations
1	Structure and Stability of Water Clusters (H2O)n, n = 8â^'20:â€‰ An Ab Initio Investigation. Journal of Physical Chemistry A, 2001, 105, 10525-10537.	2.5	459
2	Significant progress in predicting the crystal structures of small organic molecules â€“ a report on the fourth blind test. Acta Crystallographica Section B: Structural Science, 2009, 65, 107-125.	1.8	371
3	Molecular tailoring approach for geometry optimization of large molecules: Energy evaluation and parallelization strategies. Journal of Chemical Physics, 2006, 125, 104109.	3.0	246
4	Some novel characteristics of atomic information entropies. Physical Review A, 1985, 32, 2602-2606.	2.5	241
5	Molecular electrostatic potentials: A topographical study. Journal of Chemical Physics, 1992, 96, 5253-5260.	3.0	204
6	Maximal and minimal characteristics of molecular electrostatic potentials. Journal of Chemical Physics, 1990, 93, 1770-1773.	3.0	179
7	Shapes and sizes of molecular anions via topographical analysis of electrostatic potential. Journal of Chemical Physics, 1991, 94, 4384-4390.	3.0	174
8	Molecular Tailoring Approach for Simulation of Electrostatic Properties. The Journal of Physical Chemistry, 1994, 98, 9165-9169.	2.9	173
9	Quantum Chemical Investigations on Molecular Clusters. Chemical Reviews, 2014, 114, 12132-12173.	47.7	170
10	Ab initio quality one-electron properties of large molecules: Development and testing of molecular tailoring approach. Journal of Computational Chemistry, 2003, 24, 484-495.	3.3	133
11	Clar's Aromatic Sextet Theory Revisited via Molecular Electrostatic Potential Topography. Journal of Organic Chemistry, 1999, 64, 2505-2512.	3.2	127
12	Information entropy and Thomas-Fermi theory. Physical Review A, 1984, 30, 620-621.	2.5	117
13	Ab Initio Structure and Vibrational Frequencies of (CF3SO2)2N-Li+Ion Pairs. Journal of Physical Chemistry A, 1999, 103, 7474-7480.	2.5	110
14	Topography of molecular scalar fields. I. Algorithm and PoincarÃ©â€“Hopf relation. Journal of Chemical Physics, 2003, 119, 5037-5043.	3.0	110
15	Intramolecular Hydrogen Bonding and Cooperative Interactions in Carbohydrates via the Molecular Tailoring Approach. Journal of Physical Chemistry A, 2008, 112, 312-321.	2.5	109
16	Molecular electrostatics. A comprehensive topographical approach. Chemical Physics Letters, 1992, 200, 373-378.	2.6	106
17	Molecular Tailoring Approach: A Route for ab Initio Treatment of Large Clusters. Accounts of Chemical Research, 2014, 47, 2739-2747.	15.6	103
18	Electronegativities of the elements from simple .CHI..alpha. theory. Journal of the American Chemical Society, 1980, 102, 2945-2948.	13.7	97

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19	A Novel Electrostatic Approach to Substituent Constants:Â Doubly Substituted Benzenes. Journal of the American Chemical Society, 1998, 120, 7049-7055.	13.7	95
20	Molecular electrostatics for probing lone pairâ€“Ï€ interactions. Physical Chemistry Chemical Physics, 2013, 15, 18401.	2.8	94
21	Estimation of Intramolecular Hydrogen Bond Energy via Molecular Tailoring Approach. Journal of Physical Chemistry A, 2006, 110, 12519-12523.	2.5	93
22	Electrostatic Potential Minimum of the Aromatic Ring as a Measure of Substituent Constant. Journal of Physical Chemistry A, 2007, 111, 710-714.	2.5	91
23	Lone Pairs: An Electrostatic Viewpoint. Journal of Physical Chemistry A, 2014, 118, 526-532.	2.5	89
24	Rigorous relationships among quantum-mechanical kinetic energy and atomic information entropies: Upper and lower bounds. Physical Review A, 1987, 36, 1932-1935.	2.5	85
25	Hâ‹Ï€ Complexes of Acetyleneâ‹Ethylene:â€‰ A Matrix Isolation and Computational Study. Journal of Physical Chemistry A, 2002, 106, 1504-1510.	2.5	85
26	Estimation of Nâ‹HÂ·Â·Â·Oâ•€ Intramolecular Hydrogen Bond Energy in Polypeptides. Journal of Physical Chemistry A, 2009, 113, 7927-7932.	2.5	84
27	Electronic Perturbations of the Aromatic Nucleus:Â Hammett Constants and Electrostatic Potential Topographyâ€. Journal of Organic Chemistry, 1997, 62, 2625-2627.	3.2	82
28	Electrostatic Potential Topology for Probing Molecular Structure, Bonding and Reactivity. Molecules, 2021, 26, 3289.	3.8	79
29	Enabling ab initio Hessian and frequency calculations of large molecules. Journal of Chemical Physics, 2008, 129, 234101.	3.0	78
30	Complementary Electrostatics for the Study of DNA Base-Pair Interactions. Journal of Physical Chemistry B, 1997, 101, 3298-3303.	2.6	76
31	Electrostatics for Exploring Hydration Patterns of Molecules. 3. Uracil. Journal of Physical Chemistry A, 2000, 104, 8976-8982.	2.5	74
32	Ab initioinvestigation of benzene clusters: Molecular tailoring approach. Journal of Chemical Physics, 2010, 133, 164308.	3.0	73
33	MOLECULAR TAILORING APPROACH: TOWARDS PC-BASED AB INITIO TREATMENT OF LARGE MOLECULES. Journal of Theoretical and Computational Chemistry, 2006, 05, 835-855.	1.8	72
34	Tailoring approach for exploring electron densities and electrostatic potentials of molecular crystals. Theoretical Chemistry Accounts, 2004, 111, 255-263.	1.4	71
35	Facilitating Minima Search for Large Water Clusters at the MP2 Level via Molecular Tailoring. Journal of Physical Chemistry Letters, 2012, 3, 2253-2258.	4.6	69
36	Intramolecular Hydrogen Bond Energy in Polyhydroxy Systems:â€‰ A Critical Comparison of Molecular Tailoring and Isodesmic Approaches. Journal of Physical Chemistry A, 2007, 111, 6472-6480.	2.5	67

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37	Revisiting Markovnikov Addition to Alkenes via Molecular Electrostatic Potential. Journal of Organic Chemistry, 2001, 66, 6883-6890.	3.2	66
38	Bounds for Coulomb energies. Journal of Chemical Physics, 1980, 72, 1034-1038.	3.0	64
39	Maximization of atomic information-entropy sum in configuration and momentum spaces. International Journal of Quantum Chemistry, 1985, 28, 311-314.	2.0	64
40	Molecular Electrostatic Potential and Electron Density Topography:â€‰ Structure and Reactivity of (substituted arene)Cr(CO)3 Complexes. Organometallics, 2000, 19, 3008-3015.	2.3	63
41	Hâ‹Ï€ complexes of acetyleneâ€“benzene: a matrix isolation and computational study. Journal of Molecular Structure, 2002, 613, 209-222.	3.6	63
42	Many-body interaction analysis: Algorithm development and application to large molecular clusters. Journal of Chemical Physics, 2004, 121, 5043-5050.	3.0	61
43	Structure, Reactivity and Aromaticity of Acenes and Their BN Analogues: A Density Functional and Electrostatic Investigation. Inorganic Chemistry, 2004, 43, 5824-5832.	4.0	61
44	Basis set dependence of the molecular electrostatic potential topography. A case study of substituted benzenes. Chemical Physics Letters, 1995, 239, 273-281.	2.6	60
45	Molecular tailoring approach in conjunction with MP2 and Riâ€MP2 codes: A comparison with fragment molecular orbital method. Journal of Computational Chemistry, 2010, 31, 2405-2418.	3.3	59
46	Use of molecular electrostatic potential for quantitative assessment of inductive effect. Physical Chemistry Chemical Physics, 2008, 10, 6492.	2.8	58
47	Patterns in hydrogen bonding via electrostatic potential topography. Journal of Chemical Physics, 1997, 107, 5625-5626.	3.0	57
48	Electrostatic Insights into the Molecular Hydration Process: A Case Study of Crown Ethersâ€. Journal of Physical Chemistry A, 1998, 102, 9987-9992.	2.5	57
49	On the applicability of fragmentation methods to conjugated Ï€ systems within density functional framework. Journal of Chemical Physics, 2010, 132, 094102.	3.0	55
50	Structure and Stability of DNA Base Trimers:Â An Electrostatic Approach. Journal of Physical Chemistry B, 1997, 101, 9657-9662.	2.6	54
51	Appraisal of molecular tailoring approach for large clusters. Journal of Chemical Physics, 2013, 138, 104101.	3.0	54
52	Does a Stacked DNA Base Pair Hydrate Better than a Hydrogen-Bonded One?:Â An ab Initio Study. Journal of Physical Chemistry A, 2000, 104, 10887-10894.	2.5	53
53	Molecular electrostatic potentials of divalent carbon(0) compounds. Physical Chemistry Chemical Physics, 2008, 10, 2298.	2.8	52
54	Deriving chemical parameters from electrostatic potential maps of molecular anions. Inorganic Chemistry, 1992, 31, 2279-2281.	4.0	51

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55	Direct and reverse transformations between electron density and electron momentum density. Physical Review A, 1981, 24, 2906-2912.	2.5	50
56	DAMQT 2.1.0: A new version of the DAMQT package enabled with the topographical analysis of electron density and electrostatic potential in molecules. Journal of Computational Chemistry, 2015, 36, 2350-2359.	3.3	47
57	Estimation of <pâ‰³ and <pâˆ’1â‰³ from atomic electron densities. Journal of Chemical Physics, 1981, 74, 5925-5926.	3.0	46
58	Effect of matrix on IR frequencies of acetylene and acetylene-methanol complex: Infrared matrix isolation and ab initio study. Journal of Chemical Physics, 2007, 127, 104501.	3.0	46
59	Intramolecular hydrogen bond energy and cooperative interactions in Î±â€‚Î²â€‚and Î³â€cyclodextrin conformers. Journal of Computational Chemistry, 2011, 32, 2996-3004.	3.3	46
60	A general parallel solution to the integral transformation and secondâ€•order Mo/llerâ€“Plesset energy evaluation on distributed memory parallel machines. Journal of Chemical Physics, 1994, 100, 1303-1307.	3.0	45
61	Molecular cluster building algorithm: Electrostatic guidelines and molecular tailoring approach. Journal of Chemical Physics, 2011, 134, 084111.	3.0	45
62	Analysis of atomic electron momentum densities: Use of information entropies in coordinate and momentum space. Chemical Physics Letters, 1985, 117, 138-142.	2.6	43
63	Electrophilic Additions to 7-Methylenenorbornenes and 7-Isopropylidenenorbornenes: Can Remote Substituents Swamp Electrostatic Control of .pi.-face Selectivity?. Journal of Organic Chemistry, 1994, 59, 1953-1955.	3.2	43
64	An information theoretic synthesis and analysis of Compton profiles. Journal of Chemical Physics, 1981, 75, 4626-4635.	3.0	42
65	Exploring Hydration Patterns of Aldehydes and Amides:Â Ab Initio Investigations. Journal of Physical Chemistry A, 2004, 108, 2492-2498.	2.5	41
66	On the monotonicity of the atomic electron momentum density and shell structure of the radial momentum density. Journal of Chemical Physics, 1983, 78, 4581-4584.	3.0	38
67	Electrostatic Potential as a Harbinger of Cation Coordination:Â CF3SO3-Ion as a Model Example. Journal of Physical Chemistry A, 1997, 101, 5678-5686.	2.5	37
68	Hydrogen Bond Energies and Cooperativity in Substituted Calix[n]arenes (n = 4, 5). Journal of Physical Chemistry A, 2012, 116, 3739-3744.	2.5	37
69	Electrostatics for probing lone pairs and their interactions. Journal of Computational Chemistry, 2018, 39, 488-499.	3.3	37
70	An application of information theory to Compton profiles. Journal of Chemical Physics, 1979, 71, 4321-4323.	3.0	36
71	Molecular interpretation of water structuring and destructuring effects: Hydration of alkanediols. Journal of Chemical Physics, 2004, 121, 12402.	3.0	36
72	Structure, Energetics, and Reactivity of Boric Acid Nanotubes: A Molecular Tailoring Approach. Journal of Physical Chemistry A, 2008, 112, 7699-7704.	2.5	36

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73	Appraisal of Through-Bond and Through-Space Substituent Effects via Molecular Electrostatic Potential Topography. Journal of Physical Chemistry A, 2010, 114, 12330-12333.	2.5	35
74	On the basic homogeneity characteristic of atomic and molecular electronic energies. Journal of Chemical Physics, 1980, 72, 3669-3673.	3.0	34
75	Electrostatic vs. Orbital Control of Facial Selectivities in ? Systems: Experimental and Theoretical Study of Electrophilic Additions to 7-Isopropylidenenorbornanes. Angewandte Chemie International Edition in English, 1994, 33, 1390-1392.	4.4	34
76	An appraisal of PoincarÃ©â€“Hopf relation and application to topography of molecular electrostatic potentials. Journal of Chemical Physics, 2008, 129, 174103.	3.0	34
77	Direct and Reliable Method for Estimating the Hydrogen Bond Energies and Cooperativity in Water Clusters, W_n, n = 3 to 8. Journal of Physical Chemistry A, 2020, 124, 6699-6706.	2.5	34
78	Some rigorous inequalities among the Weizsacker correction and atomic ã€ˆrnã€‰ and ã€ˆpnã€‰ values. Journal of Chemical Physics, 1986, 84, 7051-7052.	3.0	33
79	An ab initio investigation on (CO2)n and CO2(Ar)m clusters: Geometries and IR spectra. Journal of Chemical Physics, 2008, 128, 124310.	3.0	33
80	Vibrational infrared and Raman spectra of polypeptides: Fragments-in-fragments within molecular tailoring approach. Journal of Chemical Physics, 2016, 144, 114113.	3.0	32
81	Development of a restricted Hartree?Fock program INDMOL on PARAM: A highly parallel computer. Journal of Computational Chemistry, 1993, 14, 445-451.	3.3	31
82	Toward an Accurate and Inexpensive Estimation of CCSD(T)/CBS Binding Energies of Large Water Clusters. Journal of Physical Chemistry A, 2016, 120, 5706-5714.	2.5	31
83	Hartree-Fock momentum expectation values for atoms and ions. Atomic Data and Nuclear Data Tables, 1983, 28, 477-491.	2.4	30
84	Molecular tailoring approach for exploring structures, energetics and properties of clusters. Journal of Chemical Sciences, 2010, 122, 47-56.	1.5	30
85	Molecular Tailoring Approach for the Estimation of Intramolecular Hydrogen Bond Energy. Molecules, 2021, 26, 2928.	3.8	30
86	Electrostatic Potential Topography for Exploring Electronic Reorganizations in 1,3 Dipolar Cycloadditions. Journal of Physical Chemistry A, 2007, 111, 2733-2738.	2.5	28
87	â€œGold standardâ€•coupled-cluster study of acetylene pentamers and hexamers via molecular tailoring approach. Theoretical Chemistry Accounts, 2011, 130, 491-500.	1.4	28
88	A Critical Analysis of the â€˜UGC-Approved List of Journalsâ€™. Current Science, 2018, 114, 1299.	0.8	28
89	The average electron momentum density and rigorous bounds to average electron densities for atoms and molecules. Chemical Physics Letters, 1986, 132, 535-540.	2.6	27
90	Cross-entropy minimization for refinement of Gaussian basis sets. Chemical Physics Letters, 1990, 166, 445-451.	2.6	27

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91	Molecular Electrostatics for Exploring Complexes of Carbonyl Compounds and Hydrogen Fluoride. Journal of Physical Chemistry A, 1999, 103, 3512-3517.	2.5	27
92	Stepwise Hydration of Protonated Carbonic Acid: A Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 12260-12275.	2.5	27
93	Signatures of molecular recognition from the topography of electrostatic potential. Journal of Chemical Sciences, 2009, 121, 815-821.	1.5	26
94	Local-density-functional model for atoms in momentum space. Physical Review A, 1982, 26, 3073-3077.	2.5	25
95	Closo-Boranes, -Carboranes, and -Silaboranes: A Topographical Study Using Electron Density and Molecular Electrostatic Potential. The Journal of Physical Chemistry, 1994, 98, 6445-6451.	2.9	25
96	Topology of molecular electron density and electrostatic potential with DAMQT. Computer Physics Communications, 2017, 214, 207-215.	7.5	25
97	Some inequalities among expectation values of oneâ€electron operators in atomic systems. Journal of Chemical Physics, 1979, 71, 1510-1510.	3.0	24
98	Polarization-Corrected Electrostatic Potential for Probing Cation Binding Patterns of Molecules. 1. Saturated Hydrocarbons. Journal of the American Chemical Society, 1998, 120, 7056-7062.	13.7	24
99	Why Are Carborane Acids so Acidic? An Electrostatic Interpretation of BrÃ¸nsted Acid Strengths. Inorganic Chemistry, 2005, 44, 9613-9615.	4.0	24
100	Lower bounds to the WeizsÃcker correction. Physical Review A, 1982, 25, 668-670.	2.5	23
101	Electrostatic guidelines and molecular tailoring for density functional investigation of structures and energetics of (Li)n clusters. Journal of Chemical Physics, 2008, 129, 164314.	3.0	23
102	Topography of Scalar Fields: Molecular Clusters and Ï€-Conjugated Systems. Journal of Physical Chemistry A, 2011, 115, 12769-12779.	2.5	23
103	Low energy isomers of (H2O)25 from a hierarchical method based on Monte Carlo temperature basin paving and molecular tailoring approaches benchmarked by MP2 calculations. Journal of Chemical Physics, 2014, 141, 164304.	3.0	23
104	Molecular Recognition via Electrostatic Potential Topography. Theoretical and Computational Chemistry, 1996, 3, 219-255.	0.4	23
105	From molecular electron density to electron momentum density. Physical Review A, 1984, 29, 3402-3405.	2.5	22
106	On the similarity between molecular electron densities, electrostatic potentials and bare nuclear potentials. Chemical Physics Letters, 1986, 130, 515-521.	2.6	22
107	Information Theoretical Approaches to Quantum Chemistry. , 2002, , 108-147.		22
108	Some investigations of symmetry and extremal properties of molecular electron momentum densities. Journal of Chemical Physics, 1991, 94, 8040-8046.	3.0	21

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109	Topographical Analysis of Electron Density and Molecular Electrostatic Potential for Cyclopropa- and Cyclobutabenzenes. Journal of the American Chemical Society, 1995, 117, 9559-9563.	13.7	21
110	Rapid topography mapping of scalar fields: Large molecular clusters. Journal of Chemical Physics, 2012, 137, 074116.	3.0	21
111	Structures, energetics and vibrational spectra of CO2 clusters through molecular tailoring and cluster building algorithm. Physical Chemistry Chemical Physics, 2012, 14, 7718.	2.8	21
112	A general parallel algorithm for the generation of moleular electrostatic potential maps. Chemical Physics Letters, 1990, 175, 307-312.	2.6	20
113	Electron localization in molecules. A comparative study of scalar fields. Computational and Theoretical Chemistry, 1996, 361, 83-91.	1.5	20
114	Accurate vibrational spectra via molecular tailoring approach: A case study of water clusters at MP2 level. Journal of Chemical Physics, 2015, 142, 014107.	3.0	20
115	Breaking the bottleneck: Use of molecular tailoring approach for the estimation of binding energies at MP2/CBS limit for large water clusters. Journal of Chemical Physics, 2016, 144, 104102.	3.0	20
116	Inequalities among atomic expectation values. Journal of Chemical Physics, 1981, 74, 589-591.	3.0	19
117	Bounds to Atomic and Molecular Energy Functionals. Advances in Quantum Chemistry, 1991, 22, 211-300.	0.8	19
118	Topographical view of molecular electron-momentum densities. Physical Review A, 1992, 45, 4399-4406.	2.5	19
119	Structure, energetics and bonding of diacetylene complexes with hydrogen fluoride. A theoretical investigation. Chemical Physics Letters, 1995, 247, 95-100.	2.6	19
120	Cation-Ï€ interaction: to stack or to spread. Molecular Physics, 2008, 106, 1557-1566.	1.7	19
121	Ab initio study on (CO₂)_nclusters via electrostaticsâ€•and molecular tailoringâ€based algorithm. International Journal of Quantum Chemistry, 2009, 109, 2238-2247.	2.0	19
122	On the Topography of Electron Momentum Densities of Linear Molecules. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1993, 48, 145-150.	1.5	18
123	Structures, energetics and vibrational spectra of (H₂O)₃₂clusters: a journey from model potentials to correlated theory. Molecular Physics, 2015, 113, 2970-2979.	1.7	18
124	Application of rigorous bounds for efficient evaluation of molecular electrostatic potentials. Chemical Physics Letters, 1990, 170, 271-276.	2.6	17
125	Topography-driven electrostatic charge models for molecules. Chemical Physics Letters, 1993, 204, 350-358.	2.6	17
126	Exploring the Gradient Paths and Zero Flux Surfaces of Molecular Electrostatic Potential. Journal of Chemical Theory and Computation, 2016, 12, 1705-1713.	5.3	17

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127	On representation of electronâ€“electron repulsion energies by simple oneâ€electron functionals. Journal of Chemical Physics, 1983, 78, 996-999.	3.0	16
128	Theoretical investigations on structure, electrostatic potentials and vibrational frequencies of diglyme and Li+â€“(diglyme) conformers. Chemical Physics Letters, 2001, 344, 527-535.	2.6	16
129	Acetylene aggregates via cluster-building algorithm and molecular tailoring approach. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	16
130	Molecular Tailoring Approach for Estimating Individual Intermolecular Interaction Energies in Benzene Clusters. Journal of Physical Chemistry A, 2021, 125, 6131-6140.	2.5	16
131	Unusually Large Hydrogen-Bond Cooperativity in Hydrogen Fluoride Clusters, (HF)_n,n= 3 to 8, Revealed by the Molecular Tailoring Approach. Journal of Physical Chemistry A, 2021, 125, 8836-8845.	2.5	16
132	On the monotonicity of atomic momentum densities and inequalities among atomic expectation values. Journal of Chemical Physics, 1982, 76, 748-749.	3.0	15
133	Relationships between the terms in the gradient expansion: Kinetic and exchange energy functionals. Physical Review A, 1982, 25, 3426-3428.	2.5	15
134	Reply to the comment on: Maximal and minimal characteristics of molecular electrostatic potentials: Some further extensions. Journal of Chemical Physics, 1991, 94, 8639-8639.	3.0	15
135	WebMTA: A webâ€interface for ab initio geometry optimization of large molecules using molecular tailoring approach. Journal of Computational Chemistry, 2009, 30, 1167-1173.	3.3	15
136	On the electrostatic nature of electrides. Physical Chemistry Chemical Physics, 2015, 17, 15030-15035.	2.8	15
137	Harmonizing accuracy and efficiency: A pragmatic approach to fragmentation of large molecules. Journal of Chemical Physics, 2018, 149, 064112.	3.0	15
138	The self-interaction correction to the local spin density model: Effect on atomic momentum space properties. Chemical Physics Letters, 1985, 120, 101-105.	2.6	14
139	Probing chemical reactions in momentum space. Journal of the American Chemical Society, 1993, 115, 7434-7438.	13.7	14
140	Use of a nonlocal density approximation for transformation from electron density to electron momentum density. Journal of Chemical Physics, 1987, 86, 2224-2228.	3.0	13
141	Reduced first-order density matrices and â€˜â€˜exchange-onlyâ€™â€™ correlation factors for some closed-shell atomic systems. Physical Review A, 1989, 40, 4224-4231.	2.5	13
142	Face selectivity in electrophilic additions to methylenenorsnoutanes: relative importance of through-space, through-bond and electrostatic interactions. Chemical Communications, 1998, , 975-976.	4.1	13
143	WebProp: Web interface forab initiocalculation of molecular oneâ€electron properties. Journal of Computational Chemistry, 2008, 29, 488-495.	3.3	13
144	PAREMD: A parallel program for the evaluation of momentum space properties of atoms and molecules. Computer Physics Communications, 2018, 224, 299-310.	7.5	13

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145	Direct and reverse transformations between electron density and electron momentum density: Connection with the locally averaged method. Physical Review A, 1983, 28, 462-463.	2.5	12
146	Rigorous bounds to molecular electron repulsion and electrostatic potential integrals. Journal of Chemical Physics, 1989, 91, 3596-3602.	3.0	12
147	Densityâ€based electron localization function via nonlocal density approximation. Journal of Chemical Physics, 1993, 98, 3574-3576.	3.0	12
148	How reliable are topographical characteristics of Hartree-Fock level molecular electron momentum densities?. Chemical Physics Letters, 1997, 274, 255-263.	2.6	12
149	Electrophilic Additions to a 2-Methylenebicyclo[2.1.1]hexane System:â€‰ Probing Ï€-Face Selectivity for Electrostatic and Orbital Effects. Organic Letters, 2002, 4, 2297-2300.	4.6	12
150	Atoms-in-molecules in momentum space: A Hirshfeld partitioning of electron momentum densities. Journal of Chemical Physics, 2006, 124, 204113.	3.0	12
151	Fragmentation method reveals a wide spectrum of intramolecular hydrogen bond energies in antioxidant natural products. New Journal of Chemistry, 2020, 44, 5841-5849.	2.8	12
152	Estimation of ã€ˆPã€‰ and ã€ˆPâ^'1ã€‰ from atomic electron densities: A comment. Journal of Chemical Physics, 1982, 77, 1073-1073.	3.0	11
153	Use of energy constraint for refinement of electron momentum distributions. Journal of Chemical Physics, 1984, 80, 1175-1178.	3.0	11
154	Interconnections between atomic-electron density and electron-momentum density: Leading and tail corrections. Physical Review A, 1986, 33, 1374-1377.	2.5	11
155	Exploring Structures and Energetics of Large OCS Clusters by Correlated Methods. Journal of Physical Chemistry A, 2013, 117, 10964-10972.	2.5	11
156	Pragmatic Many-Body Approach for Economic MP2 Energy Estimation of Molecular Clusters. Journal of Physical Chemistry A, 2019, 123, 5005-5011.	2.5	11
157	Computation of molecular electrostatic potential: An efficient algorithm and parallelization. Computers & Chemistry, 1991, 15, 203-206.	1.2	10
158	Is corannulene a better diene or dienophile? A DFT analysis. Journal of Physical Organic Chemistry, 2008, 21, 146-154.	1.9	10
159	Quantum chemical and electrostatic studies of anionic water clusters, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si17.gif" overflow="scroll"><mml:mrow><mml:mmultiscripts><mml:mrow><mml:msub><mml:mrow><mml:mtext>(H</mml:mtext></mml:mrow /><mml:none /><mml:mrow><mml:mo>-</mml:mo></mml:mrow></mml:mmultiscripts></mml:mrow></mml:math>. Computational and Theoretical Chemistry, 2008, 851, 213-219.	1.5	10
160	High-Level ab Initio Investigations on Structures and Energetics of N₂O Clusters. Journal of Physical Chemistry A, 2013, 117, 8591-8598.	2.5	10
161	Antiaromaticityâ€“Aromaticity Interplay in Fused Benzenoid Systems Using Molecular Electrostatic Potential Topology. Journal of Physical Chemistry A, 2021, 125, 5999-6012.	2.5	10
162	A â€œcriticalâ€•appraisal of electrostatic charge models for molecules. Journal of Chemical Sciences, 1994, 106, 303-314.	1.5	10

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163	Gradient-free representation of the WeizsÃcker term for atoms. Physical Review A, 1983, 28, 1808-1809.	2.5	9
164	Electron density to electron momentum density: The use of an energy constraint. Physical Review A, 1983, 27, 3328-3331.	2.5	9
165	Adsorption of water on sodium chloride surfaces: electrostatics â€“ guided ab initio studies. Theoretical Chemistry Accounts, 2005, 114, 129-136.	1.4	9
166	Hybrid QTAIM and electrostatic potential-based quantum topology phase diagrams for water clusters. Physical Chemistry Chemical Physics, 2015, 17, 15258-15273.	2.8	9
167	Bonding and Reactivity Patterns from Electrostatic Landscapes of Molecules. Journal of Chemical Sciences, 2016, 128, 1519-1526.	1.5	9
168	Electrostatic Topographical Viewpoint of Ï€-Conjugation and Aromaticity of Hydrocarbons. Journal of Physical Chemistry A, 2019, 123, 10139-10151.	2.5	9
169	Radii of monopositive atomic ions. Journal of Chemical Physics, 1993, 99, 3149-3150.	3.0	8
170	Can Ring Strain Be Realized in Momentum Space?. Journal of the American Chemical Society, 2006, 128, 10702-10706.	13.7	8
171	Hydration shell model for expeditious and reliable individual hydrogen bond energies in large water clusters. Physical Chemistry Chemical Physics, 2022, 24, 15462-15473.	2.8	8
172	On representation of Coulomb integral by oneâ€electron functionals. Journal of Chemical Physics, 1981, 75, 4740-4741.	3.0	7
173	Coulomb energy, total X-ray scattering intensities and average electron densities. Chemical Physics Letters, 1987, 142, 205-208.	2.6	7
174	Molecular electrostatic charge models: A topographical approach. International Journal of Quantum Chemistry, 1994, 49, 397-407.	2.0	7
175	Personal computer-based visualization of three-dimensional scalar and vector fields: An application to molecular graphics. Journal of Molecular Graphics, 1996, 14, 19-22.	1.1	7
176	Topography of Atomic and Molecular Scalar Fields. Computational Chemistry - Reviews of Current Trends, 1999, , 1-53.	0.4	7
177	Tailoring approach for obtaining molecular orbitals of large systems#. Journal of Chemical Sciences, 2012, 124, 149-158.	1.5	7
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