Angel MartÃ-n PendÃ¡s

List of Publications by Year
in descending order

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208	9,084	50170	46693
papers	citations	46	89
		h-index	g-index

227	227	227	4511
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Interacting Quantum Atoms:Â A Correlated Energy Decomposition Scheme Based on the Quantum Theory of Atoms in Molecules. Journal of Chemical Theory and Computation, 2005, 1, 1096-1109.	2.3	632
2	Thermodynamical properties of solids from microscopic theory: applications to MgF2 and Al2O3. Computational and Theoretical Chemistry, 1996, 368, 245-255.	1.5	523
3	First-principles study of the rocksaltâ€“cesium chloride relative phase stability in alkali halides. Physical Review B, 2002, 66, .	1.1	484
4	Quantum-Mechanical Study of Thermodynamic and Bonding Properties of MgF2. Journal of Physical Chemistry A, 1998, 102, 1595-1601.	1.1	410
5	Critic: a new program for the topological analysis of solid-state electron densities. Computer Physics Communications, 2009, 180, 157-166.	3.0	307
6	Bond Paths as Privileged Exchange Channels. Chemistry - A European Journal, 2007, 13, 9362-9371.	1.7	297
7	A Molecular Energy Decomposition Scheme for Atoms in Molecules. Journal of Chemical Theory and Computation, 2006, 2, 90-102.	2.3	271
8	The nature of the hydrogen bond: A synthesis from the interacting quantum atoms picture. Journal of Chemical Physics, 2006, 125, 184112.	1.2	208
9	A Classification of Covalent, Ionic, and Metallic Solids Based on the Electron Density. Journal of the American Chemical Society, 2002, 124, 14721-14723.	6.6	160
10	Two-electron integrations in the quantum theory of atoms in molecules. Journal of Chemical Physics, 2004, 120, 4581-4592.	1.2	157
11	Non-nuclear Maxima of the Electron Density. Physical Review Letters, 1999, 83, 1930-1933.	2.9	155
12	Extension of the interacting quantum atoms (IQA) approach to B3LYP level density functional theory (DFT). Physical Chemistry Chemical Physics, 2016, 18, 20986-21000.	1.3	140
13	Chemical fragments in real space: Definitions, properties, and energetic decompositions. Journal of Computational Chemistry, 2007, 28, 161-184.	1.5	138
14	Local compressibilities in crystals. Physical Review B, 2000, 62, 13970-13978.	1.1	130
15	Ions in crystals: The topology of the electron density in ionic materials. I. Fundamentals. Physical Review B, 1997, 55, 4275-4284.	1.1	125
16	Revitalizing the concept of bond order through delocalization measures in real space. Chemical Science, 2018, 9, 5517-5529.	3.7	114
17	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	1.5	113
18	Ions in crystals: The topology of the electron density in ionic materials.II. The cubic alkali halide perovskites. Physical Review B, 1997, 55, 4285-4297.	1.1	110

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19	Hydrogen bond cooperativity and anticooperativity within the water hexamer. Physical Chemistry Chemical Physics, 2016, 18, 19557-19566.	1.3	106
20	Ions in Crystals:â€‰ The Topology of the Electron Density in Ionic Materials. III. Geometry and Ionic Radii. Journal of Physical Chemistry B, 1998, 102, 6937-6948.	1.2	100
21	Bonding between strongly repulsive metal atoms: an oxymoron made real in a confined space of endohedral metallofullerenes. Chemical Communications, 2012, 48, 8031.	2.2	99
22	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	1.1	99
23	Theoretical explanation of the uniform compressibility behavior observed in oxide spinels. Physical Review B, 2001, 63, .	1.1	96
24	Two-electron integrations in the Quantum Theory of Atoms in Molecules with correlated wave functions. Journal of Computational Chemistry, 2005, 26, 344-351.	1.5	92
25	Binding Energies of First Row Diatomics in the Light of the Interacting Quantum Atoms Approach. Journal of Physical Chemistry A, 2006, 110, 12864-12869.	1.1	91
26	Domainâ€Averaged Exchangeâ€Correlation Energies as a Physical Underpinning for Chemical Graphs. ChemPhysChem, 2013, 14, 1211-1218.	1.0	89
27	Pressure-inducedB1-B2 phase transition in alkali halides: General aspects from first-principles calculations. Physical Review B, 1994, 49, 3066-3074.	1.1	82
28	Bonding in Classical and Nonclassical Transition Metal Carbonyls: The Interacting Quantum Atoms Perspective. Journal of Chemical Theory and Computation, 2010, 6, 1064-1074.	2.3	80
29	Hydrogenâ€Bond Cooperative Effects in Small Cyclic Water Clusters as Revealed by the Interacting Quantum Atoms Approach. Chemistry - A European Journal, 2013, 19, 14304-14315.	1.7	80
30	Steric repulsions, rotation barriers, and stereoelectronic effects: A real space perspective. Journal of Computational Chemistry, 2009, 30, 98-109.	1.5	78
31	Chemical Bonding in Group III Nitrides. Journal of the American Chemical Society, 2002, 124, 4116-4123.	6.6	75
32	Rigorous characterization of oxygen vacancies in ionic oxides. Physical Review B, 2002, 66, .	1.1	75
33	Dative and Electronâ€Sharing Bonding in C₂F₄. Chemistry - A European Journal, 2018, 24, 9083-9089.	1.7	73
34	Electron number probability distributions for correlated wave functions. Journal of Chemical Physics, 2007, 126, 094102.	1.2	69
35	Quantum-mechanical analysis of the equation of state of anataseTiO2. Physical Review B, 2001, 64, .	1.1	68
36	Interacting Quantum Atomsâ€”A Review. Molecules, 2020, 25, 4028.	1.7	67

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37	The nature of resonance-assisted hydrogen bonds: a quantum chemical topology perspective. Physical Chemistry Chemical Physics, 2016, 18, 26383-26390.	1.3	64
38	An electron number distribution view of chemical bonds in real space. Physical Chemistry Chemical Physics, 2007, 9, 1087-1092.	1.3	59
39	The Ehrenfest force field: Topology and consequences for the definition of an atom in a molecule. Journal of Chemical Physics, 2012, 137, 134101.	1.2	59
40	Topological Analysis of Chemical Bonding in Cyclophosphazenes. Journal of Physical Chemistry A, 2001, 105, 5280-5291.	1.1	57
41	Generalized Huzinaga buildingâ€block equations for nonorthogonal electronic groups: Relation to the Adamsâ€“Gilbert theory. Journal of Chemical Physics, 1992, 97, 6504-6508.	1.2	54
42	Non-nuclear maxima of the electron density on alkaline metals. Journal of Chemical Physics, 2003, 119, 6341-6350.	1.2	54
43	Stress, virial, and pressure in the theory of atoms in molecules. Journal of Chemical Physics, 2002, 117, 965-979.	1.2	51
44	Bond metallicity of materials from real space charge density distributions. Chemical Physics Letters, 2009, 471, 174-177.	1.2	51
45	Nature of Chemical Interactions from the Profiles of Electron Delocalization Indices. Journal of Chemical Theory and Computation, 2011, 7, 1704-1711.	2.3	51
46	Partitioning the DFT exchange-correlation energy in line with the interacting quantum atoms approach. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	50
47	Low- and high-pressureab initioequations of state for the alkali chlorides. Physical Review B, 1993, 48, 5891-5901.	1.1	47
48	First Principles Study of Polyatomic Clusters of AlN, GaN, and InN. 2. Chemical Bonding. Journal of Physical Chemistry B, 2000, 104, 4368-4374.	1.2	47
49	Spin resolved electron number distribution functions: How spins couple in real space. Journal of Chemical Physics, 2007, 127, 144103.	1.2	47
50	Oneâ€electron images in real space: Natural adaptive orbitals. Journal of Computational Chemistry, 2015, 36, 833-843.	1.5	46
51	Quantum mechanical cluster calculations of ionic materials: the ab initio perturbed ion (version 7) program. Computer Physics Communications, 1993, 77, 107-134.	3.0	43
52	Pauling Resonant Structures in Real Space through Electron Number Probability Distributions. Journal of Physical Chemistry A, 2007, 111, 1084-1090.	1.1	43
53	EDF: Computing electron number probability distribution functions in real space from molecular wave functions. Computer Physics Communications, 2008, 178, 621-634.	3.0	43
54	Hirshfeld surfaces as approximations to interatomic surfaces. Journal of Chemical Physics, 2002, 117, 1017-1023.	1.2	41

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55	Evolution of the Properties of AlnNnClusters with Size. Journal of Physical Chemistry B, 2005, 109, 24352-24360.	1.2	40
56	Charge transfer, chemical potentials, and the nature of functional groups: answers from quantum chemical topology. Faraday Discussions, 2007, 135, 423-438.	1.6	40
57	A multipolar approach to the interatomic covalent interaction energy. Journal of Computational Chemistry, 2017, 38, 816-829.	1.5	40
58	Dynamical correlation within the Interacting Quantum Atoms method through coupled cluster theory. Computational and Theoretical Chemistry, 2015, 1053, 90-95.	1.1	39
59	Restoring orbital thinking from real space descriptions: bonding in classical and non-classical transition metal carbonyls. Physical Chemistry Chemical Physics, 2011, 13, 5068.	1.3	37
60	A hierarchy of chemical bonding indices in real space from reduced density matrices and cumulants. Computational and Theoretical Chemistry, 2013, 1003, 71-78.	1.1	37
61	Ions in Crystals:â€‰ The Topology of the Electron Density in Ionic Materials. 4. The Danburite (CaB2Si2O8) Case and the Occurrence of Oxideâ"Oxide Bond Paths in Crystals. Journal of Physical Chemistry B, 2003, 107, 4912-4921.	1.2	36
62	First Principles Study of Neutral and Anionic (Medium-Size) Aluminum Nitride Clusters:Â AlnNn,n= 7â"16. Journal of Physical Chemistry B, 2006, 110, 4092-4098.	1.2	36
63	Beyond the molecular orbital conception of electronically excited states through the quantum theory of atoms in molecules. Physical Chemistry Chemical Physics, 2014, 16, 9249-9258.	1.3	36
64	Performance of the Density Matrix Functional Theory in the Quantum Theory of Atoms in Molecules. Journal of Physical Chemistry A, 2012, 116, 1237-1250.	1.1	35
65	Electron correlation in the interacting quantum atoms partition via coupledâ€cluster lagrangian densities. Journal of Computational Chemistry, 2016, 37, 1753-1765.	1.5	32
66	Universal Features of the Topological Bond Properties of the Electron Density. Journal of Physical Chemistry A, 2004, 108, 2794-2801.	1.1	31
67	Unusual substituent effects on the bonding of iminoboranes. Physical Chemistry Chemical Physics, 2007, 9, 3970-3977.	1.3	31
68	Bond Order Densities in Real Space. Journal of Physical Chemistry A, 2020, 124, 339-352.	1.1	31
69	Electronâ€"electron interactions between ELF basins. Chemical Physics Letters, 2008, 454, 396-403.	1.2	30
70	Toward Understanding the Photochemistry of Photoactive Yellow Protein: A CASPT2/CASSCF and Quantum Theory of Atoms in Molecules Combined Study of a Model Chromophore in Vacuo. Journal of Chemical Theory and Computation, 2009, 5, 3032-3038.	2.3	30
71	Cooperative and anticooperative effects in resonance assisted hydrogen bonds in merged structures of malondialdehyde. Physical Chemistry Chemical Physics, 2017, 19, 97-107.	1.3	30
72	On Electrostatics, Covalency, and Chemical Dashes: Physical Interactions versus Chemical Bonds. Chemistry - A European Journal, 2019, 25, 309-314.	1.7	30

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73	A connection between domain-averaged Fermi hole orbitals and electron number distribution functions in real space. Journal of Chemical Physics, 2009, 131, 124125.	1.2	29
74	Understanding the bifurcated halogen bonding Nâ‹¯Halâ‹¯N in bidentate diazaheterocyclic compounds. Computational and Theoretical Chemistry, 2015, 1053, 229-237.	1.1	29
75	Chemical bonding in excited states: Energy transfer and charge redistribution from a real space perspective. Journal of Computational Chemistry, 2017, 38, 957-970.	1.5	29
76	Polarity inversion in the electron density of BP crystal. Physical Review B, 2001, 63, .	1.1	28
77	Structural and chemical stability of halide perovskites. Solid State Communications, 1997, 104, 47-50.	0.9	27
78	Static simulations ofCaF2polymorphs. Physical Review B, 1994, 49, 5858-5868.	1.1	26
79	How Electron Localization Function Quantifies and Pictures Chemical Changes in a Solid: The B3 â†' B1 Pressure Induced Phase Transition in BeO. Journal of Physical Chemistry B, 2008, 112, 9787-9794.	1.2	26
80	Computation of Local and Global Properties of the Electron Localization Function Topology in Crystals. Journal of Chemical Theory and Computation, 2009, 5, 164-173.	2.3	26
81	Useful applications of the electron localization function in high-pressure crystal chemistry. Journal of Physics and Chemistry of Solids, 2008, 69, 2204-2207.	1.9	25
82	Using Pseudopotentials within the Interacting Quantum Atoms Approach. Journal of Physical Chemistry A, 2009, 113, 7963-7971.	1.1	24
83	On the interpretation of domain averaged Fermi hole analyses of correlated wavefunctions. Physical Chemistry Chemical Physics, 2014, 16, 4586.	1.3	24
84	The bifunctional catalytic role of water clusters in the formation of acid rain. Chemical Communications, 2017, 53, 3516-3519.	2.2	24
85	Where Does Electron Correlation Lie? Some Answers from a Real Space Partition. ChemPhysChem, 2017, 18, 3553-3561.	1.0	24
86	Ab initio cluster-in-the-lattice description of vanadium-doped zircon: analysis of the impurity centers in vanadium(4+)-doped zircon (ZrSiO4). The Journal of Physical Chemistry, 1993, 97, 2555-2559.	2.9	23
87	Derivation of electron-gas interatomic potentials from quantum-mechanical descriptions of ions in crystals. Physical Review B, 1995, 51, 2703-2714.	1.1	23
88	Ions in crystals: The topology of the electron density in ionic materials. V. TheB1â^'B2phase transition in alkali halides. Physical Review B, 2000, 62, 12028-12039.	1.1	23
89	A view of covalent and ionic bonding from Maximum Probability Domains. Computational and Theoretical Chemistry, 2015, 1053, 142-149.	1.1	23
90	Chemical Bonding from the Statistics of the Electron Distribution. ChemPhysChem, 2019, 20, 2722-2741.	1.0	22

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91	Challenging the electrostatic Ïƒâ€hole picture of halogen bonding using minimal models and the interacting quantum atoms approach. Journal of Computational Chemistry, 2021, 42, 676-687.	1.5	22
92	Energy Partition Analyses: Symmetry-Adapted Perturbation Theory and Other Techniques. , 2017, , 27-64.		21
93	Application of the Interacting Quantum Atoms Approach to the S66 and Ionicâ€Hydrogenâ€Bond Datasets for Noncovalent Interactions. ChemPhysChem, 2018, 19, 973-987.	1.0	21
94	Spatial localization, correlation, and statistical dependence of electrons in atomic domains: The <mml:math altimg="si10.gif" display="inline" 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="h. Chemical Physics Letters, 200	1.2	20
95	An anatomy of intramolecular atomic interactions in halogen-substituted trinitromethanes. Physical Chemistry Chemical Physics, 2014, 16, 16780-16789.	1.3	20
96	An Interacting Quantum Atoms Analysis of the Metalâ€“Metal Bond in [M₂(CO)₈]ⁿ Systems. Journal of Physical Chemistry A, 2015, 119, 2153-2160.	1.1	20
97	Hydrogenâ€Bond Weakening through Ïƒ Systems: Resonanceâ€Impaired Hydrogen Bonds (RIHB). Chemistry - A European Journal, 2017, 23, 16605-16611.	1.7	20
98	Realâ€Space In Situ Bond Energies: Toward A Consistent Energetic Definition of Bond Strength. Chemistry - A European Journal, 2018, 24, 9101-9112.	1.7	20
99	Beryllium Bonding in the Light of Modern Quantum Chemical Topology Tools. Journal of Physical Chemistry A, 2018, 122, 849-858.	1.1	20
100	Real space bond orders are energetic descriptors. Physical Chemistry Chemical Physics, 2018, 20, 16231-16237.	1.3	20
101	Halogen Bonds in Clathrate Cages: A Real Space Perspective. ChemPhysChem, 2018, 19, 2512-2517.	1.0	20
102	On the strength of hydrogen bonding within water clusters on the coordination limit. Journal of Computational Chemistry, 2020, 41, 2266-2277.	1.5	20
103	Collective interactions among organometallics are exotic bonds hidden on lab shelves. Nature Communications, 2022, 13, 2069.	5.8	20
104	Universal-binding-energy relations across the rock-saltâ€“cesium chloride phase transition in alkali halides. Physical Review B, 1997, 56, 3010-3015.	1.1	19
105	Revisiting the variational nature of the quantum theory of atoms in molecules. Chemical Physics Letters, 2006, 417, 16-21.	1.2	19
106	The Nature of the Interaction of Organoselenium Molecules with Diiodine. Journal of Physical Chemistry A, 2011, 115, 10069-10077.	1.1	19
107	Electron number distribution functions from molecular wavefunctions. Version 2. Computer Physics Communications, 2014, 185, 2663-2682.	3.0	19
108	Convergence of the multipole expansion for 1,2 Coulomb interactions: The modified multipole shifting algorithm. Journal of Chemical Physics, 2010, 132, 194110.	1.2	18

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109	The rotational barrier of ethane and some of its hexasubstituted derivatives in terms of the forces acting on the electron distribution. Physical Chemistry Chemical Physics, 2015, 17, 19021-19029.	1.3	17
110	Fermi and Coulomb correlation effects upon the interacting quantum atoms energy partition. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	17
111	Partition of electronic excitation energies: the IQA/EOM-CCSD method. Physical Chemistry Chemical Physics, 2019, 21, 13428-13439.	1.3	17
112	Energetic Descriptors of Steric Hindrance in Real Space: An Improved IQA Picture**. ChemPhysChem, 2021, 22, 775-787.	1.0	17
113	Microscopic analysis of the compressibility in the spinel phase of Si 3 N 4. Europhysics Letters, 2001, 54, 760-766.	0.7	16
114	Comparison of Direct and Flow Integration Based Charge Density Population Analyses. Journal of Physical Chemistry A, 2007, 111, 12146-12151.	1.1	16
115	An unexpected bridge between chemical bonding indicators and electrical conductivity through the localization tensor. Physical Chemistry Chemical Physics, 2017, 19, 1790-1797.	1.3	16
116	A chemical theory of topological insulators. Chemical Communications, 2019, 55, 12281-12287.	2.2	16
117	Quantum Chemical Topology as a Theory of Open Quantum Systems. Journal of Chemical Theory and Computation, 2019, 15, 1079-1088.	2.3	16
118	Efficient implementation of the interacting quantum atoms energy partition of the secondâ€•order MÃ¸llerâ€“Plesset energy. Journal of Computational Chemistry, 2020, 41, 1234-1241.	1.5	16
119	On the Relationship between Hydrogen Bond Strength and the Formation Energy in Resonance-Assisted Hydrogen Bonds. Molecules, 2021, 26, 4196.	1.7	16
120	Anti-ohmic single molecule electron transport: is it feasible?. Nanoscale Advances, 2019, 1, 1901-1913.	2.2	15
121	Structure and Bonding in Magnesium Difluoride Clusters:Â The (MgF2)n(n= 2â^'3) Clusters. Journal of Physical Chemistry A, 2002, 106, 335-344.	1.1	14
122	Global optimization of ionic MgnF2n (n=1â€“30) clusters. Journal of Chemical Physics, 2005, 123, 234305.	1.2	14
123	Decay Rate of Correlated Real-Space Delocalization Measures: Insights into Chemical Bonding and Mott Transitions from Hydrogen Chains. Journal of Chemical Theory and Computation, 2016, 12, 3053-3062.	2.3	14
124	Decay rate of real space delocalization measures: a comparison between analytical and test systems. Physical Chemistry Chemical Physics, 2016, 18, 11772-11780.	1.3	14
125	Decoding real space bonding descriptors in valence bond language. Physical Chemistry Chemical Physics, 2018, 20, 12368-12372.	1.3	14
126	Overlap, effective-potential, and projection-operator bicentric integrals over complex Slater-type orbitals. Physical Review A, 1991, 43, 3384-3391.	1.0	13

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127	Bases for Understanding Polymerization under Pressure: The Practical Case of CO₂. Journal of Physical Chemistry B, 2009, 113, 1068-1073.	1.2	13
128	Assessing the Reversed Exponential Decay of the Electrical Conductance in Molecular Wires: The Undeniable Effect of Static Electron Correlation. Nano Letters, 2019, 19, 7394-7399.	4.5	13
129	Fluorine conformational effects characterized by energy decomposition analysis. Physical Chemistry Chemical Physics, 2019, 21, 25258-25275.	1.3	13
130	Directing the Crystal Packing in Triphenylphosphine Gold(I) Thiolates by Ligand Fluorination. Inorganic Chemistry, 2020, 59, 8667-8677.	1.9	13
131	Ab initio pair potentials from quantum-mechanical atoms-in-crystals calculations. Journal of Physics Condensed Matter, 1993, 5, 4975-4988.	0.7	12
132	Generalized electron number distribution functions: real space versus orbital space descriptions. Theoretical Chemistry Accounts, 2011, 128, 433-444.	0.5	12
133	Quantitative Electron Delocalization in Solids from Maximally Localized Wannier Functions. Journal of Chemical Theory and Computation, 2018, 14, 4699-4710.	2.3	12
134	Structure and Bonding in Magnesium Difluoride Clusters:Â The MgF2Molecule. Journal of Physical Chemistry A, 2001, 105, 4126-4135.	1.1	11
135	Chemical Interactions and Spin Structure in (O₂)₄: Implications for the Îµ-O₂ Phase. Journal of Chemical Theory and Computation, 2013, 9, 2179-2188.	2.3	11
136	A first step towards quantum energy potentials of electron pairs. Physical Chemistry Chemical Physics, 2019, 21, 4215-4223.	1.3	11
137	Laplacian of the Hamiltonian Kinetic Energy Density as an Indicator of Binding and Weak Interactions. ChemPhysChem, 2020, 21, 194-203.	1.0	11
138	Exotic Bonding Regimes Uncovered in Excited States. Chemistry - A European Journal, 2019, 25, 12169-12179.	1.7	10
139	Tetrel Interactions from an Interacting Quantum Atoms Perspective. Molecules, 2019, 24, 2204.	1.7	10
140	Local spin and open quantum systems: clarifying misconceptions, unifying approaches. Physical Chemistry Chemical Physics, 2021, 23, 8375-8392.	1.3	10
141	Atomistic simulation of the pressure-temperature-volume diagram in Î±-Al2O3. Solid State Communications, 1996, 98, 41-44.	0.9	9
142	Topological properties of the electron density of solids and molecules. Recent developments in Oviedo. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, 434-437.	0.3	9
143	Efficient algorithms for Hirshfeld-I charges. Journal of Chemical Physics, 2015, 143, 084115.	1.2	9
144	How Electronic Excitation Can be Used to Inhibit Some Mechanisms Associated to Substituent Effects. ChemPhysChem, 2016, 17, 2666-2671.	1.0	9

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145	Ï€-Backbonding and non-covalent interactions in the JohnPhos and polyfluorothiolate complexes of gold(<scp>i</scp>). Dalton Transactions, 2017, 46, 12456-12465.	1.6	9
146	Curvature of interatomic surfaces. I. Fundamentals. Journal of Chemical Physics, 2003, 119, 7633-7642.	1.2	8
147	Bonding and compressibility in molecular and polymeric phases of solid CO2. Journal of Physics Condensed Matter, 2004, 16, S1263-S1270.	0.7	8
148	Electron number distribution functions with iterative Hirshfeld atoms. Computational and Theoretical Chemistry, 2011, 975, 2-8.	1.1	8
149	Emergent Scalar and Vector Fields in Quantum Chemical Topology. Challenges and Advances in Computational Chemistry and Physics, 2016, , 131-150.	0.6	8
150	From quantum fragments to Lewis structures: electron counting in position space. Physical Chemistry Chemical Physics, 2018, 20, 21368-21380.	1.3	8
151	Photochemistry in Real Space: Bathoâ€•and Hypsochromism in the Water Dimer. Chemistry - A European Journal, 2020, 26, 17035-17045.	1.7	8
152	Electronic structure and electronic excitations of solid neon from an ab initio atom-in-the-lattice approach. The Journal of Physical Chemistry, 1992, 96, 2301-2307.	2.9	7
153	Modeling theO2â^'-O2â^'interaction for atomistic simulations. Physical Review B, 1995, 51, 11289-11295.	1.1	7
154	Ionic properties of perovskites derived from topological analysis of their wave function. Journal of Physics Condensed Matter, 1999, 11, 6329-6336.	0.7	7
155	Curvature of interatomic surfaces. II. Origin and systematics. Journal of Chemical Physics, 2003, 119, 7643-7650.	1.2	7
156	Structural effects of trifluoromethylation and fluorination in gold(<scp>i</scp>) BIPHEP fluorothiolates. New Journal of Chemistry, 2017, 41, 10537-10541.	1.4	7
157	The Activation Strain Model in the Light of Real Space Energy Partitions. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2020, 646, 1062-1072.	0.6	7
158	Interacting Quantum Atoms Analysis of the Reaction Force: A Tool to Analyze Driving and Retarding Forces in Chemical Reactions. ChemPhysChem, 2021, 22, 1976-1988.	1.0	7
159	Interacting Quantum Atoms Method for Crystalline Solids. Journal of Physical Chemistry A, 2021, 125, 9011-9025.	1.1	7
160	Stronger-together: the cooperativity of aurophilic interactions. Chemical Communications, 2022, 58, 1398-1401.	2.2	7
161	Beyond Standard Charge Density Topological Analyses. , 2011, , 303-358.		6
162	Perspectives for quantum chemical topology in crystallography. Physica Scripta, 2013, 87, 048106.	1.2	6

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163	On the stability of some analytically solvable maximum probability domains. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	6
164	Performance of the RI and RIJCOSX approximations in the topological analysis of the electron density. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	6
165	Stability and trans Influence in Fluorinated Gold(I) Coordination Compounds. European Journal of Inorganic Chemistry, 2018, 2018, 4413-4420.	1.0	6
166	Lewis Structures from Open Quantum Systems Natural Orbitals: Real Space Adaptive Natural Density Partitioning. Journal of Physical Chemistry A, 2021, 125, 4013-4025.	1.1	6
167	QM/MM Energy Decomposition Using the Interacting Quantum Atoms Approach. Journal of Chemical Information and Modeling, 2022, 62, 1510-1524.	2.5	6
168	Does Steric Hindrance Actually Govern the Competition between Bimolecular Substitution and Elimination Reactions?. Journal of Physical Chemistry A, 2022, 126, 1871-1880.	1.1	6
169	The role of references and the elusive nature of the chemical bond. Nature Communications, 2022, 13, .	5.8	6
170	Exact versus truncated spectrally resolved exchange in ab initio calculations. Journal of Chemical Physics, 1992, 97, 452-458.	1.2	5
171	Inference of crystal properties from cluster magnitudes. Journal of Chemical Physics, 1995, 103, 432-439.	1.2	5
172	Reply to comments of Bader on the simplified variational derivation for quantum atoms in molecules. Chemical Physics Letters, 2006, 426, 229-230.	1.2	5
173	Theoretical Simulation of AlN Nanocrystals. Journal of Physical Chemistry C, 2008, 112, 6667-6676.	1.5	5
174	Interacting Quantum Atoms Approach and Electrostatic Solvation Energy: Assessing Atomic and Group Solvation Contributions. ChemPhysChem, 2018, 19, 3425-3435.	1.0	5
175	Electron-pair bonding in real space. Is the charge-shift family supported?. Chemical Communications, 2019, 55, 5071-5074.	2.2	5
176	NNAIMQ: A neural network model for predicting QTAIM charges. Journal of Chemical Physics, 2022, 156, 014112.	1.2	5
177	Universal compressibility behaviour of ions in ionic crystals. High Pressure Research, 2009, 29, 97-102.	0.4	4
178	Hierarchies of quantum chemical descriptors induced by statistical analyses of domain occupation number operators. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1456.	6.2	4
179	Electronegativity equalization: taming an old problem with new tools. Physical Chemistry Chemical Physics, 2020, 22, 22880-22884.	1.3	4
180	Energetics of Electron Pairs in Electrophilic Aromatic Substitutions. Molecules, 2021, 26, 513.	1.7	4

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