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	Questioning the orbital picture of magnetic spin coupling: a real space alternative. Physical Chemistry Chemical Physics, 2022, 24, 639-652.	1.3	2
2	Stronger-together: the cooperativity of aurophilic interactions. Chemical Communications, 2022, 58, 1398-1401.	2.2	7
3	NNAIMQ: A neural network model for predicting QTAIM charges. Journal of Chemical Physics, 2022, 156, 014112.	1.2	5
4	QM/MM Energy Decomposition Using the Interacting Quantum Atoms Approach. Journal of Chemical Information and Modeling, 2022, 62, 1510-1524.	2.5	6
5	A real space picture of the role of steric effects in <scp> S _N 2 </scp> reactions. Journal of Computational Chemistry, 2022, 43, 785-795.	1.5	4
6	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
7	Atomic shell structure from Born probabilities: Comparison to other shell descriptors and persistence in molecules. Journal of Chemical Physics, 2022, 156, 164103.	1.2	4
8	Collective interactions among organometallics are exotic bonds hidden on lab shelves. Nature Communications, 2022, 13, 2069.	5.8	20
9	The role of references and the elusive nature of the chemical bond. Nature Communications, 2022, 13, .	5.8	6
10	The nature of the intermolecular interaction in (H2X)2 (X = O, S, Se). Physical Chemistry Chemical Physics, 2021, 23, 10097-10107.	1.3	3
11	Local spin and open quantum systems: clarifying misconceptions, unifying approaches. Physical Chemistry Chemical Physics, 2021, 23, 8375-8392.	1.3	10
12	Energetics of Electron Pairs in Electrophilic Aromatic Substitutions. Molecules, 2021, 26, 513.	1.7	4
13	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
14	Energetic Descriptors of Steric Hindrance in Real Space: An Improved IQA Picture**. ChemPhysChem, 2021, 22, 775-787.	1.0	17
15	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
16	Understanding Topological Insulators in Real Space. Molecules, 2021, 26, 2965.	1.7	1
17	On the Relationship between Hydrogen Bond Strength and the Formation Energy in Resonance-Assisted Hydrogen Bonds. Molecules, 2021, 26, 4196.	1.7	16
18	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

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19	Interacting Quantum Atoms Method for Crystalline Solids. Journal of Physical Chemistry A, 2021, 125, 9011-9025.	1.1	7
20	Implementation of the interacting quantum atom energy decomposition using the CASPT2 method. Physical Chemistry Chemical Physics, 2021, 23, 27508-27519.	1.3	4
21	Laplacian of the Hamiltonian Kinetic Energy Density as an Indicator of Binding and Weak Interactions. ChemPhysChem, 2020, 21, 194-203.	1.0	11
22	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
23	Bond Order Densities in Real Space. Journal of Physical Chemistry A, 2020, 124, 339-352.	1.1	31
24	DFT performance in the IQA energy partition of small water clusters. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	2
25	Electronegativity equalization: taming an old problem with new tools. Physical Chemistry Chemical Physics, 2020, 22, 22880-22884.	1.3	4
26	On the strength of hydrogen bonding within water clusters on the coordination limit. Journal of Computational Chemistry, 2020, 41, 2266-2277.	1.5	20
27	Interacting Quantum Atomsâ€”A Review. Molecules, 2020, 25, 4028.	1.7	67
28	Photochemistry in Real Space: Bathoâ€•and Hypsochromism in the Water Dimer. Chemistry - A European Journal, 2020, 26, 17035-17045.	1.7	8
29	Photochemistry in Real Space: Bathoâ€•and Hypsochromism in the Water Dimer. Chemistry - A European Journal, 2020, 26, 16951-16951.	1.7	0
30	Directing the Crystal Packing in Triphenylphosphine Gold(I) Thiolates by Ligand Fluorination. Inorganic Chemistry, 2020, 59, 8667-8677.	1.9	13
31	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
32	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
33	Exotic Bonding Regimes Uncovered in Excited States. Chemistry - A European Journal, 2019, 25, 12169-12179.	1.7	10
34	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	1.5	113
35	Tetrel Interactions from an Interacting Quantum Atoms Perspective. Molecules, 2019, 24, 2204.	1.7	10
36	Chemical Bonding from the Statistics of the Electron Distribution. ChemPhysChem, 2019, 20, 2722-2741.	1.0	22

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37	On the impact of a phosphoryl group in the recognition capabilities of 2-aminopyridines toward carboxylic acids. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	1
38	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
39	A chemical theory of topological insulators. Chemical Communications, 2019, 55, 12281-12287.	2.2	16
40	A first step towards quantum energy potentials of electron pairs. Physical Chemistry Chemical Physics, 2019, 21, 4215-4223.	1.3	11
41	Mimicking Enzymes: Asymmetric Induction inside a Carbamateâ€“Based Steroidal Cleft. Organic Letters, 2019, 21, 3994-3997.	2.4	3
42	Partition of electronic excitation energies: the IQA/EOM-CCSD method. Physical Chemistry Chemical Physics, 2019, 21, 13428-13439.	1.3	17
43	Reply to the â€˜Comment on â€œDecoding real space bonding descriptors in valence bond languageâ€â€™ by S. Shaik, P. Hiberty and D. Danovich, Phys. Chem. Chem. Phys., 2019, 21, DOI: 10.1039/C8CP07225F. Physical Chemistry Chemical Physics, 2019, 21, 8175-8178.	1.3	1
44	Anti-ohmic single molecule electron transport: is it feasible?. Nanoscale Advances, 2019, 1, 1901-1913.	2.2	15
45	Electron-pair bonding in real space. Is the charge-shift family supported?. Chemical Communications, 2019, 55, 5071-5074.	2.2	5
46	Fluorine conformational effects characterized by energy decomposition analysis. Physical Chemistry Chemical Physics, 2019, 21, 25258-25275.	1.3	13
47	Quantum Chemical Topology as a Theory of Open Quantum Systems. Journal of Chemical Theory and Computation, 2019, 15, 1079-1088.	2.3	16
48	On Electrostatics, Covalency, and Chemical Dashes: Physical Interactions versus Chemical Bonds. Chemistry - A European Journal, 2019, 25, 309-314.	1.7	30
49	Decoding real space bonding descriptors in valence bond language. Physical Chemistry Chemical Physics, 2018, 20, 12368-12372.	1.3	14
50	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
51	Dative and Electronâ€Sharing Bonding in C₂F₄. Chemistry - A European Journal, 2018, 24, 9083-9089.	1.7	73
52	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
53	Beryllium Bonding in the Light of Modern Quantum Chemical Topology Tools. Journal of Physical Chemistry A, 2018, 122, 849-858.	1.1	20
54	Interacting Quantum Atoms Approach and Electrostatic Solvation Energy: Assessing Atomic and Group Solvation Contributions. ChemPhysChem, 2018, 19, 3425-3435.	1.0	5

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55	Stability and trans Influence in Fluorinated Gold(I) Coordination Compounds. European Journal of Inorganic Chemistry, 2018, 2018, 4413-4420.	1.0	6
56	Real space bond orders are energetic descriptors. Physical Chemistry Chemical Physics, 2018, 20, 16231-16237.	1.3	20
57	Halogen Bonds in Clathrate Cages: A Real Space Perspective. ChemPhysChem, 2018, 19, 2512-2517.	1.0	20
58	Quantitative Electron Delocalization in Solids from Maximally Localized Wannier Functions. Journal of Chemical Theory and Computation, 2018, 14, 4699-4710.	2.3	12
59	From quantum fragments to Lewis structures: electron counting in position space. Physical Chemistry Chemical Physics, 2018, 20, 21368-21380.	1.3	8
60	Revitalizing the concept of bond order through delocalization measures in real space. Chemical Science, 2018, 9, 5517-5529.	3.7	114
61	A multipolar approach to the interatomic covalent interaction energy. Journal of Computational Chemistry, 2017, 38, 816-829.	1.5	40
62	The bifunctional catalytic role of water clusters in the formation of acid rain. Chemical Communications, 2017, 53, 3516-3519.	2.2	24
63	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
64	Performance of the RI and RIJCOSX approximations in the topological analysis of the electron density. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	6
65	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
66	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
67	Where Does Electron Correlation Lie? Some Answers from a Real Space Partition. ChemPhysChem, 2017, 18, 3553-3561.	1.0	24
68	Electron sharing and localization in real space for the Mott transition from 1RDMFT periodic calculations. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	0
69	Structural effects of trifluoromethylation and fluorination in gold(<scp>i</scp>) BIPHEP fluorothiolates. New Journal of Chemistry, 2017, 41, 10537-10541.	1.4	7
70	Hydrogenâ€Bond Weakening through Ï€ Systems: Resonanceâ€Impaired Hydrogen Bonds (RIHB). Chemistry - A European Journal, 2017, 23, 16605-16611.	1.7	20
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	Energy Partition Analyses: Symmetry-Adapted Perturbation Theory and Other Techniques. , 2017, , 27-64.		21

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73	The nature of resonance-assisted hydrogen bonds: a quantum chemical topology perspective. Physical Chemistry Chemical Physics, 2016, 18, 26383-26390.	1.3	64
74	Partitioning the DFT exchange-correlation energy in line with the interacting quantum atoms approach. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	50
75	Electron correlation in the interacting quantum atoms partition via coupledâ€cluster lagrangian densities. Journal of Computational Chemistry, 2016, 37, 1753-1765.	1.5	32
76	Hydrogen bond cooperativity and anticooperativity within the water hexamer. Physical Chemistry Chemical Physics, 2016, 18, 19557-19566.	1.3	106
77	Emergent Scalar and Vector Fields in Quantum Chemical Topology. Challenges and Advances in Computational Chemistry and Physics, 2016, , 131-150.	0.6	8
78	Fermi and Coulomb correlation effects upon the interacting quantum atoms energy partition. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	17
79	How Electronic Excitation Can be Used to Inhibit Some Mechanisms Associated to Substituent Effects. ChemPhysChem, 2016, 17, 2666-2671.	1.0	9
80	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
81	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
82	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
83	Towards an energy partition into real space resonance structures: 1- and 2-particle density matrix decomposition. Molecular Physics, 2016, 114, 1334-1344.	0.8	3
84	Efficient algorithms for Hirshfeld-I charges. Journal of Chemical Physics, 2015, 143, 084115.	1.2	9
85	Oneâ€electron images in real space: Natural adaptive orbitals. Journal of Computational Chemistry, 2015, 36, 833-843.	1.5	46
86	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
87	Preface to the Special Issue on â€œUnderstanding structure and reactivity from topology and beyondâ€. Computational and Theoretical Chemistry, 2015, 1053, 1.	1.1	1
88	Revisiting the carbonyl n â†' Ï€* electronic excitation through topological eyes: expanding, enriching and enhancing the chemical language using electron number distribution functions and domain averaged Fermi holes. Physical Chemistry Chemical Physics, 2015, 17, 26059-26071.	1.3	3
89	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
90	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	1.1	99

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91	Dynamical correlation within the Interacting Quantum Atoms method through coupled cluster theory. Computational and Theoretical Chemistry, 2015, 1053, 90-95.	1.1	39
92	A view of covalent and ionic bonding from Maximum Probability Domains. Computational and Theoretical Chemistry, 2015, 1053, 142-149.	1.1	23
93	Understanding the bifurcated halogen bonding Nâ‹¯Halâ‹¯N in bidentate diazaheterocyclic compounds. Computational and Theoretical Chemistry, 2015, 1053, 229-237.	1.1	29
94	An anatomy of intramolecular atomic interactions in halogen-substituted trinitromethanes. Physical Chemistry Chemical Physics, 2014, 16, 16780-16789.	1.3	20
95	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
96	On the stability of some analytically solvable maximum probability domains. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	6
97	On the interpretation of domain averaged Fermi hole analyses of correlated wavefunctions. Physical Chemistry Chemical Physics, 2014, 16, 4586.	1.3	24
98	Electron number distribution functions from molecular wavefunctions. Version 2. Computer Physics Communications, 2014, 185, 2663-2682.	3.0	19
99	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
100	Perspectives for quantum chemical topology in crystallography. Physica Scripta, 2013, 87, 048106.	1.2	6
101	Domainâ€Averaged Exchangeâ€Correlation Energies as a Physical Underpinning for Chemical Graphs. ChemPhysChem, 2013, 14, 1211-1218.	1.0	89
102	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
103	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
104	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
105	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
106	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
107	Beyond Standard Charge Density Topological Analyses. , 2011, , 303-358.		6
108	Nature of Chemical Interactions from the Profiles of Electron Delocalization Indices. Journal of Chemical Theory and Computation, 2011, 7, 1704-1711.	2.3	51

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109	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
110	Electron number distribution functions with iterative Hirshfeld atoms. Computational and Theoretical Chemistry, 2011, 975, 2-8.	1.1	8
111	The Nature of the Interaction of Organoselenium Molecules with Diiodine. Journal of Physical Chemistry A, 2011, 115, 10069-10077.	1.1	19
112	Generalized electron number distribution functions: real space versus orbital space descriptions. Theoretical Chemistry Accounts, 2011, 128, 433-444.	0.5	12
113	Is a more predictable QTAIM possible?. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C99-C99.	0.3	0
114	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
115	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
116	Universal compressibility behaviour of ions in ionic crystals. High Pressure Research, 2009, 29, 97-102.	0.4	4
117	Steric repulsions, rotation barriers, and stereoelectronic effects: A real space perspective. Journal of Computational Chemistry, 2009, 30, 98-109.	1.5	78
118	Critic: a new program for the topological analysis of solid-state electron densities. Computer Physics Communications, 2009, 180, 157-166.	3.0	307
119	Bond metallicity of materials from real space charge density distributions. Chemical Physics Letters, 2009, 471, 174-177.	1.2	51
120	Bases for Understanding Polymerization under Pressure: The Practical Case of CO₂. Journal of Physical Chemistry B, 2009, 113, 1068-1073.	1.2	13
121	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
122	Using Pseudopotentials within the Interacting Quantum Atoms Approach. Journal of Physical Chemistry A, 2009, 113, 7963-7971.	1.1	24
123	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
124	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
125	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
126	EDF: Computing electron number probability distribution functions in real space from molecular wave functions. Computer Physics Communications, 2008, 178, 621-634.	3.0	43

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127	Electronâ€“electron interactions between ELF basins. Chemical Physics Letters, 2008, 454, 396-403.	1.2	30
128	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
129	Theoretical Simulation of AlN Nanocrystals. Journal of Physical Chemistry C, 2008, 112, 6667-6676.	1.5	5
130	Pauling Resonant Structures in Real Space through Electron Number Probability Distributions. Journal of Physical Chemistry A, 2007, 111, 1084-1090.	1.1	43
131	An electron number distribution view of chemical bonds in real space. Physical Chemistry Chemical Physics, 2007, 9, 1087-1092.	1.3	59
132	Comparison of Direct and Flow Integration Based Charge Density Population Analyses. Journal of Physical Chemistry A, 2007, 111, 12146-12151.	1.1	16
133	Spin resolved electron number distribution functions: How spins couple in real space. Journal of Chemical Physics, 2007, 127, 144103.	1.2	47
134	Charge transfer, chemical potentials, and the nature of functional groups: answers from quantum chemical topology. Faraday Discussions, 2007, 135, 423-438.	1.6	40
135	Unusual substituent effects on the bonding of iminoboranes. Physical Chemistry Chemical Physics, 2007, 9, 3970-3977.	1.3	31
136	Bond Paths as Privileged Exchange Channels. Chemistry - A European Journal, 2007, 13, 9362-9371.	1.7	297
137	Chemical fragments in real space: Definitions, properties, and energetic decompositions. Journal of Computational Chemistry, 2007, 28, 161-184.	1.5	138
138	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
139	Electron number probability distributions for correlated wave functions. Journal of Chemical Physics, 2007, 126, 094102.	1.2	69
140	A Molecular Energy Decomposition Scheme for Atoms in Molecules. Journal of Chemical Theory and Computation, 2006, 2, 90-102.	2.3	271
141	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
142	The nature of the hydrogen bond: A synthesis from the interacting quantum atoms picture. Journal of Chemical Physics, 2006, 125, 184112.	1.2	208
143	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
144	Revisiting the variational nature of the quantum theory of atoms in molecules. Chemical Physics Letters, 2006, 417, 16-21.	1.2	19

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145	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
146	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
147	Global optimization of ionic MgnF2n (n=1â€“30) clusters. Journal of Chemical Physics, 2005, 123, 234305.	1.2	14
148	Evolution of the Properties of AlnNnClusters with Size. Journal of Physical Chemistry B, 2005, 109, 24352-24360.	1.2	40
149	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
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152	Two-electron integrations in the quantum theory of atoms in molecules. Journal of Chemical Physics, 2004, 120, 4581-4592.	1.2	157
153	Universal Features of the Topological Bond Properties of the Electron Density. Journal of Physical Chemistry A, 2004, 108, 2794-2801.	1.1	31
154	Bonding and compressibility in molecular and polymeric phases of solid CO2. Journal of Physics Condensed Matter, 2004, 16, S1263-S1270.	0.7	8
155	A Classification of Covalent, Ionic, and Metallic Solids Based on the Electron Density.. ChemInform, 2003, 34, no.	0.1	0
156	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
157	Curvature of interatomic surfaces. I. Fundamentals. Journal of Chemical Physics, 2003, 119, 7633-7642.	1.2	8
158	Curvature of interatomic surfaces. II. Origin and systematics. Journal of Chemical Physics, 2003, 119, 7643-7650.	1.2	7
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164	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
165	Stress, virial, and pressure in the theory of atoms in molecules. Journal of Chemical Physics, 2002, 117, 965-979.	1.2	51
166	Microscopic Study of the Rock Salt-Caesium Chloride Phase Stability in Alkali Halides. High Pressure Research, 2002, 22, 443-446.	0.4	1
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169	Theoretical explanation of the uniform compressibility behavior observed in oxide spinels. Physical Review B, 2001, 63, .	1.1	96
170	Structure and Bonding in Magnesium Difluoride Clusters:Â The MgF2Molecule. Journal of Physical Chemistry A, 2001, 105, 4126-4135.	1.1	11
171	Topological Analysis of Chemical Bonding in Cyclophosphazenes. Journal of Physical Chemistry A, 2001, 105, 5280-5291.	1.1	57
172	Microscopic analysis of the compressibility in the spinel phase of Si 3 N 4. Europhysics Letters, 2001, 54, 760-766.	0.7	16
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175	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
176	Local compressibilities in crystals. Physical Review B, 2000, 62, 13970-13978.	1.1	130
177	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
178	Strategies for determining and usingab initiointerionic potentials. Radiation Effects and Defects in Solids, 1999, 151, 223-228.	0.4	3
179	Ionic properties of perovskites derived from topological analysis of their wave function. Journal of Physics Condensed Matter, 1999, 11, 6329-6336.	0.7	7
180	Non-nuclear Maxima of the Electron Density. Physical Review Letters, 1999, 83, 1930-1933.	2.9	155

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