Angel Martn Pends

List of Publications by Year in Descending Order

197 papers	7,629 citations	44 h-index	81 g-index
227 ext. papers	8,311 ext. citations	3.7 avg, IF	6.09 L-index

#	Paper	IF	Citations
197	NNAIMQ: A neural network model for predicting QTAIM charges.. *Journal of Chemical Physics*, **2022**, 156, 014112	3.9	1
196	Atomic shell structure from Born probabilities: Comparison to other shell descriptors and persistence in molecules.. *Journal of Chemical Physics*, **2022**, 156, 164103	3.9	1
195	Collective interactions among organometallics are exotic bonds hidden on lab shelves.. *Nature Communications*, **2022**, 13, 2069	17.4	4
194	The role of references and the elusive nature of the chemical bond. *Nature Communications*, **2022**, 13,	17.4	2
193	Implementation of the interacting quantum atom energy decomposition using the CASPT2 method. *Physical Chemistry Chemical Physics*, **2021**,	3.6	1
192	Energetic Descriptors of Steric Hindrance in Real Space: An Improved IQA Picture*. *ChemPhysChem*, **2021**, 22, 775-787	3.2	4
191	Lewis Structures from Open Quantum Systems Natural Orbitals: Real Space Adaptive Natural Density Partitioning. *Journal of Physical Chemistry A*, **2021**, 125, 4013-4025	2.8	2
190	On the Relationship between Hydrogen Bond Strength and the Formation Energy in Resonance-Assisted Hydrogen Bonds. *Molecules*, **2021**, 26,	4.8	4
189	The nature of the intermolecular interaction in (HX) (X = O, S, Se). *Physical Chemistry Chemical Physics*, **2021**, 23, 10097-10107	3.6	2
188	Local spin and open quantum systems: clarifying misconceptions, unifying approaches. *Physical Chemistry Chemical Physics*, **2021**, 23, 8375-8392	3.6	5
187	Challenging the electrostatic hole picture of halogen bonding using minimal models and the interacting quantum atoms approach. *Journal of Computational Chemistry*, **2021**, 42, 676-687	3.5	10
186	Interacting Quantum Atoms Analysis of the Reaction Force: A Tool to Analyze Driving and Retarding Forces in Chemical Reactions. *ChemPhysChem*, **2021**, 22, 1976-1988	3.2	3
185	Interacting Quantum Atoms Method for Crystalline Solids. *Journal of Physical Chemistry A*, **2021**, 125, 9011-9025	2.8	2
184	Photochemistry in Real Space: Batho- and Hypsochromism in the Water Dimer. *Chemistry - A European Journal*, **2020**, 26, 16951	4.8	
183	Directing the Crystal Packing in Triphenylphosphine Gold(I) Thiolates by Ligand Fluorination. *Inorganic Chemistry*, **2020**, 59, 8667-8677	5.1	5
182	Efficient implementation of the interacting quantum atoms energy partition of the second-order Møller-Plesset energy. *Journal of Computational Chemistry*, **2020**, 41, 1234-1241	3.5	7
181	Laplacian of the Hamiltonian Kinetic Energy Density as an Indicator of Binding and Weak Interactions. *ChemPhysChem*, **2020**, 21, 194-203	3.2	8

180	Hierarchies of quantum chemical descriptors induced by statistical analyses of domain occupation number operators. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1456	7.9	2
179	Bond Order Densities in Real Space. *Journal of Physical Chemistry A*, **2020**, 124, 339-352	2.8	8
178	DFT performance in the IQA energy partition of small water clusters. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	2
177	Electronegativity equalization: taming an old problem with new tools. *Physical Chemistry Chemical Physics*, **2020**, 22, 22880-22884	3.6	2
176	On the strength of hydrogen bonding within water clusters on the coordination limit. *Journal of Computational Chemistry*, **2020**, 41, 2266-2277	3.5	12
175	Interacting Quantum Atoms-A Review. *Molecules*, **2020**, 25,	4.8	27
174	Photochemistry in Real Space: Batho- and Hypsochromism in the Water Dimer. *Chemistry - A European Journal*, **2020**, 26, 17035-17045	4.8	6
173	The Activation Strain Model in the Light of Real Space Energy Partitions. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2020**, 646, 1062-1072	1.3	4
172	On the impact of a phosphoryl group in the recognition capabilities of 2-aminopyridines toward carboxylic acids. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	0
171	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	11.5	9
170	A chemical theory of topological insulators. *Chemical Communications*, **2019**, 55, 12281-12287	5.8	10
169	A first step towards quantum energy potentials of electron pairs. *Physical Chemistry Chemical Physics*, **2019**, 21, 4215-4223	3.6	9
168	Mimicking Enzymes: Asymmetric Induction inside a Carbamate-Based Steroidal Cleft. *Organic Letters*, **2019**, 21, 3994-3997	6.2	3
167	Partition of electronic excitation energies: the IQA/EOM-CCSD method. *Physical Chemistry Chemical Physics*, **2019**, 21, 13428-13439	3.6	11
166	Reply to the ‘Comment on "Decoding real space bonding descriptors in valence bond language" 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	3.6	
165	Anti-ohmic single molecule electron transport: is it feasible?. *Nanoscale Advances*, **2019**, 1, 1901-1913	5.1	10
164	Electron-pair bonding in real space. Is the charge-shift family supported?. *Chemical Communications*, **2019**, 55, 5071-5074	5.8	5
163	Exotic Bonding Regimes Uncovered in Excited States. *Chemistry - A European Journal*, **2019**, 25, 12169-12179	4.8	9

162	Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, **2019**, 40, 2248-2283	3.5	70
161	Tetrel Interactions from an Interacting Quantum Atoms Perspective. *Molecules*, **2019**, 24,	4.8	7
160	Chemical Bonding from the Statistics of the Electron Distribution. *ChemPhysChem*, **2019**, 20, 2722-2741	3.2	17
159	Fluorine conformational effects characterized by energy decomposition analysis. *Physical Chemistry Chemical Physics*, **2019**, 21, 25258-25275	3.6	7
158	Quantum Chemical Topology as a Theory of Open Quantum Systems. *Journal of Chemical Theory and Computation*, **2019**, 15, 1079-1088	6.4	11
157	On Electrostatics, Covalency, and Chemical Dashes: Physical Interactions versus Chemical Bonds. *Chemistry - A European Journal*, **2019**, 25, 309-314	4.8	21
156	Decoding real space bonding descriptors in valence bond language. *Physical Chemistry Chemical Physics*, **2018**, 20, 12368-12372	3.6	10
155	Real-Space In Situ Bond Energies: Toward A Consistent Energetic Definition of Bond Strength. *Chemistry - A European Journal*, **2018**, 24, 9101-9112	4.8	16
154	Dative and Electron-Sharing Bonding in C F. *Chemistry - A European Journal*, **2018**, 24, 9083-9089	4.8	50
153	Application of the Interacting Quantum Atoms Approach to the S66 and Ionic-Hydrogen-Bond Datasets for Noncovalent Interactions. *ChemPhysChem*, **2018**, 19, 973-987	3.2	14
152	Beryllium Bonding in the Light of Modern Quantum Chemical Topology Tools. *Journal of Physical Chemistry A*, **2018**, 122, 849-858	2.8	14
151	Halogen Bonds in Clathrate Cages: A Real Space Perspective. *ChemPhysChem*, **2018**, 19, 2512-2517	3.2	18
150	Quantitative Electron Delocalization in Solids from Maximally Localized Wannier Functions. *Journal of Chemical Theory and Computation*, **2018**, 14, 4699-4710	6.4	7
149	From quantum fragments to Lewis structures: electron counting in position space. *Physical Chemistry Chemical Physics*, **2018**, 20, 21368-21380	3.6	8
148	Revitalizing the concept of bond order through delocalization measures in real space. *Chemical Science*, **2018**, 9, 5517-5529	9.4	77
147	Interacting Quantum Atoms Approach and Electrostatic Solvation Energy: Assessing Atomic and Group Solvation Contributions. *ChemPhysChem*, **2018**, 19, 3425-3435	3.2	3
146	Stability and trans Influence in Fluorinated Gold(I) Coordination Compounds. *European Journal of Inorganic Chemistry*, **2018**, 2018, 4413-4420	2.3	5
145	Real space bond orders are energetic descriptors. *Physical Chemistry Chemical Physics*, **2018**, 20, 16231-16237	3.6	16

144	A multipolar approach to the interatomic covalent interaction energy. *Journal of Computational Chemistry*, **2017**, 38, 816-829	3.5	32
143	The bifunctional catalytic role of water clusters in the formation of acid rain. *Chemical Communications*, **2017**, 53, 3516-3519	5.8	18
142	Chemical bonding in excited states: Energy transfer and charge redistribution from a real space perspective. *Journal of Computational Chemistry*, **2017**, 38, 957-970	3.5	23
141	Performance of the RI and RIJCOSX approximations in the topological analysis of the electron density. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	5
140	Backbonding and non-covalent interactions in the JohnPhos and polyfluorothiolate complexes of gold(i). *Dalton Transactions*, **2017**, 46, 12456-12465	4.3	6
139	An unexpected bridge between chemical bonding indicators and electrical conductivity through the localization tensor. *Physical Chemistry Chemical Physics*, **2017**, 19, 1790-1797	3.6	12
138	Where Does Electron Correlation Lie? Some Answers from a Real Space Partition. *ChemPhysChem*, **2017**, 18, 3553-3561	3.2	19
137	Energy Partition Analyses: Symmetry-Adapted Perturbation Theory and Other Techniques **2017**, 27-64		13
136	Electron sharing and localization in real space for the Mott transition from 1RDMFT periodic calculations. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	
135	Structural effects of trifluoromethylation and fluorination in gold(I) BIPHEP fluorothiolates. *New Journal of Chemistry*, **2017**, 41, 10537-10541	3.6	7
134	Hydrogen-Bond Weakening through systems: Resonance-Impaired Hydrogen Bonds (RIHB). *Chemistry - A European Journal*, **2017**, 23, 16605-16611	4.8	17
133	How Electronic Excitation Can be Used to Inhibit Some Mechanisms Associated to Substituent Effects. *ChemPhysChem*, **2016**, 17, 2666-71	3.2	8
132	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, 3053-62	6.4	10
131	Decay rate of real space delocalization measures: a comparison between analytical and test systems. *Physical Chemistry Chemical Physics*, **2016**, 18, 11772-80	3.6	11
130	Extension of the interacting quantum atoms (IQA) approach to B3LYP level density functional theory (DFT). *Physical Chemistry Chemical Physics*, **2016**, 18, 20986-1000	3.6	103
129	Towards an energy partition into real space resonance structures: 1- and 2-particle density matrix decomposition. *Molecular Physics*, **2016**, 114, 1334-1344	1.7	3
128	Cooperative and anticooperative effects in resonance assisted hydrogen bonds in merged structures of malondialdehyde. *Physical Chemistry Chemical Physics*, **2016**, 19, 97-107	3.6	25
127	The nature of resonance-assisted hydrogen bonds: a quantum chemical topology perspective. *Physical Chemistry Chemical Physics*, **2016**, 18, 26383-90	3.6	48

126	Partitioning the DFT exchange-correlation energy in line with the interacting quantum atoms approach. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	37
125	Electron correlation in the interacting quantum atoms partition via coupled-cluster lagrangian densities. *Journal of Computational Chemistry*, **2016**, 37, 1753-65	3.5	26
124	Hydrogen bond cooperativity and anticooperativity within the water hexamer. *Physical Chemistry Chemical Physics*, **2016**, 18, 19557-66	3.6	83
123	Emergent Scalar and Vector Fields in Quantum Chemical Topology. *Challenges and Advances in Computational Chemistry and Physics*, **2016**, 131-150	0.7	7
122	Fermi and Coulomb correlation effects upon the interacting quantum atoms energy partition. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	17
121	Revisiting the carbonyl n -> π* 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, 26059-71	3.6	3
120	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, 19021-9	3.6	14
119	Six questions on topology in theoretical chemistry. *Computational and Theoretical Chemistry*, **2015**, 1053, 2-16	2	81
118	Dynamical correlation within the Interacting Quantum Atoms method through coupled cluster theory. *Computational and Theoretical Chemistry*, **2015**, 1053, 90-95	2	33
117	A view of covalent and ionic bonding from Maximum Probability Domains. *Computational and Theoretical Chemistry*, **2015**, 1053, 142-149	2	21
116	Understanding the bifurcated halogen bonding N?Hal?N in bidentate diazaheterocyclic compounds. *Computational and Theoretical Chemistry*, **2015**, 1053, 229-237	2	27
115	Efficient algorithms for Hirshfeld-I charges. *Journal of Chemical Physics*, **2015**, 143, 084115	3.9	7
114	One-electron images in real space: natural adaptive orbitals. *Journal of Computational Chemistry*, **2015**, 36, 833-43	3.5	25
113	An interacting quantum atoms analysis of the metal-metal bond in [M2(CO)8]n systems. *Journal of Physical Chemistry A*, **2015**, 119, 2153-60	2.8	16
112	An anatomy of intramolecular atomic interactions in halogen-substituted trinitromethanes. *Physical Chemistry Chemical Physics*, **2014**, 16, 16780-9	3.6	19
111	Beyond the molecular orbital conception of electronically excited states through the quantum theory of atoms in molecules. *Physical Chemistry Chemical Physics*, **2014**, 16, 9249-58	3.6	30
110	On the stability of some analytically solvable maximum probability domains. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	5
109	On the interpretation of domain averaged Fermi hole analyses of correlated wavefunctions. *Physical Chemistry Chemical Physics*, **2014**, 16, 4586-97	3.6	23

108	Electron number distribution functions from molecular wavefunctions. Version 2. *Computer Physics Communications*, **2014**, 185, 2663-2682	4.2	18
107	Hydrogen-bond cooperative effects in small cyclic water clusters as revealed by the interacting quantum atoms approach. *Chemistry - A European Journal*, **2013**, 19, 14304-15	4.8	71
106	Perspectives for quantum chemical topology in crystallography. *Physica Scripta*, **2013**, 87, 048106	2.6	5
105	Domain-averaged exchange-correlation energies as a physical underpinning for chemical graphs. *ChemPhysChem*, **2013**, 14, 1211-8	3.2	74
104	Chemical Interactions and Spin Structure in (O2)4: Implications for the □O2 Phase. *Journal of Chemical Theory and Computation*, **2013**, 9, 2179-88	6.4	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	2	26
102	Performance of the density matrix functional theory in the quantum theory of atoms in molecules. *Journal of Physical Chemistry A*, **2012**, 116, 1237-50	2.8	32
101	The Ehrenfest force field: Topology and consequences for the definition of an atom in a molecule. *Journal of Chemical Physics*, **2012**, 137, 134101	3.9	48
100	Bonding between strongly repulsive metal atoms: an oxymoron made real in a confined space of endohedral metallofullerenes. *Chemical Communications*, **2012**, 48, 8031-50	5.8	81
99	Beyond Standard Charge Density Topological Analyses **2011**, 303-358		6
98	Nature of Chemical Interactions from the Profiles of Electron Delocalization Indices. *Journal of Chemical Theory and Computation*, **2011**, 7, 1704-11	6.4	48
97	Restoring orbital thinking from real space descriptions: bonding in classical and non-classical transition metal carbonyls. *Physical Chemistry Chemical Physics*, **2011**, 13, 5068-77	3.6	34
96	Electron number distribution functions with iterative Hirshfeld atoms. *Computational and Theoretical Chemistry*, **2011**, 975, 2-8	2	8
95	The nature of the interaction of organoselenium molecules with diiodine. *Journal of Physical Chemistry A*, **2011**, 115, 10069-77	2.8	18
94	Generalized electron number distribution functions: real space versus orbital space descriptions. *Theoretical Chemistry Accounts*, **2011**, 128, 433-444	1.9	12
93	Convergence of the multipole expansion for 1,2 Coulomb interactions: The modified multipole shifting algorithm. *Journal of Chemical Physics*, **2010**, 132, 194110	3.9	15
92	Bonding in Classical and Nonclassical Transition Metal Carbonyls: The Interacting Quantum Atoms Perspective. *Journal of Chemical Theory and Computation*, **2010**, 6, 1064-1074	6.4	68
91	Universal compressibility behaviour of ions in ionic crystals. *High Pressure Research*, **2009**, 29, 97-102	1.6	4

90	Steric repulsions, rotation barriers, and stereoelectronic effects: a real space perspective. *Journal of Computational Chemistry*, **2009**, 30, 98-109	3.5	74
89	Critic: a new program for the topological analysis of solid-state electron densities. *Computer Physics Communications*, **2009**, 180, 157-166	4.2	231
88	Bond metallicity of materials from real space charge density distributions. *Chemical Physics Letters*, **2009**, 471, 174-177	2.5	41
87	Bases for Understanding Polymerization under Pressure: The Practical Case of CO2. *Journal of Physical Chemistry B*, **2009**, 113, 1068-73	3.4	13
86	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, 3032-8	6.4	28
85	Using pseudopotentials within the interacting quantum atoms approach. *Journal of Physical Chemistry A*, **2009**, 113, 7963-71	2.8	22
84	A connection between domain-averaged Fermi hole orbitals and electron number distribution functions in real space. *Journal of Chemical Physics*, **2009**, 131, 124125	3.9	28
83	Computation of Local and Global Properties of the Electron Localization Function Topology in Crystals. *Journal of Chemical Theory and Computation*, **2009**, 5, 164-73	6.4	22
82	How electron localization function quantifies and pictures chemical changes in a solid: the B3-->B1 pressure induced phase transition in BeO. *Journal of Physical Chemistry B*, **2008**, 112, 9787-94	3.4	25
81	Theoretical Simulation of AlN Nanocrystals. *Journal of Physical Chemistry C*, **2008**, 112, 6667-6676	3.8	5
80	Useful applications of the electron localization function in high-pressure crystal chemistry. *Journal of Physics and Chemistry of Solids*, **2008**, 69, 2204-2207	3.9	24
79	EDF: Computing electron number probability distribution functions in real space from molecular wave functions. *Computer Physics Communications*, **2008**, 178, 621-634	4.2	40
78	Electron□electron interactions between ELF basins. *Chemical Physics Letters*, **2008**, 454, 396-403	2.5	26
77	An electron number distribution view of chemical bonds in real space. *Physical Chemistry Chemical Physics*, **2007**, 9, 1087-92	3.6	57
76	Comparison of direct and flow integration based charge density population analyses. *Journal of Physical Chemistry A*, **2007**, 111, 12146-51	2.8	15
75	Spin resolved electron number distribution functions: how spins couple in real space. *Journal of Chemical Physics*, **2007**, 127, 144103	3.9	46
74	Charge transfer, chemical potentials, and the nature of functional groups: answers from quantum chemical topology. *Faraday Discussions*, **2007**, 135, 423-38; discussion 489-506	3.6	36
73	Unusual substituent effects on the bonding of iminoboranes. *Physical Chemistry Chemical Physics*, **2007**, 9, 3970-7	3.6	29

72	Bond paths as privileged exchange channels. *Chemistry - A European Journal*, **2007**, 13, 9362-71	4.8	260
71	Chemical fragments in real space: definitions, properties, and energetic decompositions. *Journal of Computational Chemistry*, **2007**, 28, 161-84	3.5	119
70	Spatial localization, correlation, and statistical dependence of electrons in atomic domains: The . *Chemical Physics Letters*, **2007**, 437, 287-292	2.5	19
69	Electron number probability distributions for correlated wave functions. *Journal of Chemical Physics* , **2007**, 126, 094102	3.9	66
68	Pauling resonant structures in real space through electron number probability distributions. *Journal of Physical Chemistry A*, **2007**, 111, 1084-90	2.8	40
67	A Molecular Energy Decomposition Scheme for Atoms in Molecules. *Journal of Chemical Theory and Computation*, **2006**, 2, 90-102	6.4	232
66	First principles study of neutral and anionic (medium-size) aluminum nitride clusters: AlnNn, n=7-16. *Journal of Physical Chemistry B*, **2006**, 110, 4092-8	3.4	34
65	The nature of the hydrogen bond: a synthesis from the interacting quantum atoms picture. *Journal of Chemical Physics*, **2006**, 125, 184112	3.9	183
64	Binding energies of first row diatomics in the light of the interacting quantum atoms approach. *Journal of Physical Chemistry A*, **2006**, 110, 12864-9	2.8	83
63	Revisiting the variational nature of the quantum theory of atoms in molecules. *Chemical Physics Letters*, **2006**, 417, 16-21	2.5	17
62	Reply to comments of Bader on the simplified variational derivation for quantum atoms in molecules. *Chemical Physics Letters*, **2006**, 426, 229-230	2.5	4
61	Global optimization of ionic Mg(n)F(2n) (n=1-30) clusters. *Journal of Chemical Physics*, **2005**, 123, 234305	3.9	14
60	Evolution of the properties of Al(n)N(n) clusters with size. *Journal of Physical Chemistry B*, **2005**, 109, 24352-60	3.4	39
59	Interacting Quantum Atoms: A Correlated Energy Decomposition Scheme Based on the Quantum Theory of Atoms in Molecules. *Journal of Chemical Theory and Computation*, **2005**, 1, 1096-109	6.4	505
58	Two-electron integrations in the quantum theory of atoms in molecules with correlated wave functions. *Journal of Computational Chemistry*, **2005**, 26, 344-51	3.5	89
57	Reduced-size representations of high-quality atomic densities. The hybrid Gaussian-Exponential case. *Theoretical Chemistry Accounts*, **2004**, 112, 113	1.9	
56	Topological properties of the electron density of solids and molecules. Recent developments in Oviedo. *Acta Crystallographica Section A: Foundations and Advances*, **2004**, 60, 434-7		8
55	Two-electron integrations in the quantum theory of atoms in molecules. *Journal of Chemical Physics* , **2004**, 120, 4581-92	3.9	143

54	Universal Features of the Topological Bond Properties of the Electron Density. *Journal of Physical Chemistry A*, **2004**, 108, 2794-2801	2.8	27
53	Bonding and compressibility in molecular and polymeric phases of solid CO2. *Journal of Physics Condensed Matter*, **2004**, 16, S1263-S1270	1.8	7
52	Ions in Crystals: The Topology of the Electron Density in Ionic Materials. 4. The Danburite (CaB2Si2O8) Case and the Occurrence of Oxide□Oxide Bond Paths in Crystals. *Journal of Physical Chemistry B*, **2003**, 107, 4912-4921	3.4	33
51	Curvature of interatomic surfaces. I. Fundamentals. *Journal of Chemical Physics*, **2003**, 119, 7633-7642	3.9	6
50	Curvature of interatomic surfaces. II. Origin and systematics. *Journal of Chemical Physics*, **2003**, 119, 7643-7650	3.9	7
49	Non-nuclear maxima of the electron density on alkaline metals. *Journal of Chemical Physics*, **2003**, 119, 6341-6350	3.9	47
48	Structure and Bonding in Magnesium Difluoride Clusters: The (MgF2)n (n = 2□) Clusters. *Journal of Physical Chemistry A*, **2002**, 106, 335-344	2.8	12
47	Chemical bonding in group III nitrides. *Journal of the American Chemical Society*, **2002**, 124, 4116-23	16.4	66
46	Rigorous characterization of oxygen vacancies in ionic oxides. *Physical Review B*, **2002**, 66,	3.3	72
45	First-principles study of the rocksalt□esium chloride relative phase stability in alkali halides. *Physical Review B*, **2002**, 66,	3.3	432
44	A classification of covalent, ionic, and metallic solids based on the electron density. *Journal of the American Chemical Society*, **2002**, 124, 14721-3	16.4	150
43	Stress, virial, and pressure in the theory of atoms in molecules. *Journal of Chemical Physics*, **2002**, 117, 965-979	3.9	44
42	Microscopic Study of the Rock Salt-Caesium Chloride Phase Stability in Alkali Halides. *High Pressure Research*, **2002**, 22, 443-446	1.6	1
41	Hirshfeld surfaces as approximations to interatomic surfaces. *Journal of Chemical Physics*, **2002**, 117, 1017-1023	3.9	31
40	Microscopic analysis of the compressibility in the spinel phase of Si 3 N 4. *Europhysics Letters*, **2001**, 54, 760-766	1.6	16
39	Practical embedding for ionic materials: Crystal-adapted pseudopotentials for the MgO crystal. *Physical Review B*, **2001**, 64,	3.3	3
38	Polarity inversion in the electron density of BP crystal. *Physical Review B*, **2001**, 63,	3.3	26
37	Quantum-mechanical analysis of the equation of state of anatase TiO2. *Physical Review B*, **2001**, 64,	3.3	63

36	Theoretical explanation of the uniform compressibility behavior observed in oxide spinels. *Physical Review B*, **2001**, 63,	3.3	88
35	Structure and Bonding in Magnesium Difluoride Clusters: The MgF2 Molecule. *Journal of Physical Chemistry A*, **2001**, 105, 4126-4135	2.8	10
34	Topological Analysis of Chemical Bonding in Cyclophosphazenes. *Journal of Physical Chemistry A*, **2001**, 105, 5280-5291	2.8	53
33	Ions in crystals: The topology of the electron density in ionic materials. V. The B1B2 phase transition in alkali halides. *Physical Review B*, **2000**, 62, 12028-12039	3.3	21
32	Local compressibilities in crystals. *Physical Review B*, **2000**, 62, 13970-13978	3.3	118
31	First Principles Study of Polyatomic Clusters of AlN, GaN, and InN. 2. Chemical Bonding. *Journal of Physical Chemistry B*, **2000**, 104, 4368-4374	3.4	46
30	Strategies for determining and using ab initio interionic potentials. *Radiation Effects and Defects in Solids*, **1999**, 151, 223-228	0.9	3
29	Ionic properties of perovskites derived from topological analysis of their wave function. *Journal of Physics Condensed Matter*, **1999**, 11, 6329-6336	1.8	7
28	Non-nuclear Maxima of the Electron Density. *Physical Review Letters*, **1999**, 83, 1930-1933	7.4	137
27	Quantum-Mechanical Study of Thermodynamic and Bonding Properties of MgF2. *Journal of Physical Chemistry A*, **1998**, 102, 1595-1601	2.8	374
26	Ions in Crystals: The Topology of the Electron Density in Ionic Materials. III. Geometry and Ionic Radii. *Journal of Physical Chemistry B*, **1998**, 102, 6937-6948	3.4	90
25	Universal-binding-energy relations across the rock-salt□esium chloride phase transition in alkali halides. *Physical Review B*, **1997**, 56, 3010-3015	3.3	18
24	Ions in crystals: The topology of the electron density in ionic materials. I. Fundamentals. *Physical Review B*, **1997**, 55, 4275-4284	3.3	111
23	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	3.3	93
22	Structural and chemical stability of halide perovskites. *Solid State Communications*, **1997**, 104, 47-50	1.6	23
21	Thermodynamical properties of solids from microscopic theory: applications to MgF2 and Al2O3. *Computational and Theoretical Chemistry*, **1996**, 368, 245-255		452
20	Atomistic simulation of the pressure-temperature-volume diagram in □Al2O3. *Solid State Communications*, **1996**, 98, 41-44	1.6	7
19	Energetics of the RbF + CaF2 -> RbCaF3 solid state reaction: A first-principles study. *Radiation Effects and Defects in Solids*, **1995**, 134, 193-196	0.9	1

18	Inference of crystal properties from cluster magnitudes. *Journal of Chemical Physics*, **1995**, 103, 432-439	3.9	4
17	Modeling the O2--O2- interaction for atomistic simulations. *Physical Review B*, **1995**, 51, 11289-11295	3.3	7
16	Stability of B1 and B2 phases from electronic density topology considerations. *Radiation Effects and Defects in Solids*, **1995**, 134, 201-203	0.9	
15	Effects of a quantum crystal potential on the derivation of electron gas interionic energies. *Radiation Effects and Defects in Solids*, **1995**, 134, 197-200	0.9	
14	Derivation of electron-gas interatomic potentials from quantum-mechanical descriptions of ions in crystals. *Physical Review B*, **1995**, 51, 2703-2714	3.3	23
13	Static simulations of Cu+ centers in alkali halides. *Radiation Effects and Defects in Solids*, **1995**, 134, 47-50	0.9	2
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