Angel Martn Pends

List of Publications by Citations

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	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
196	Thermodynamical properties of solids from microscopic theory: applications to MgF2 and Al2O3. *Computational and Theoretical Chemistry*, **1996**, 368, 245-255		452
195	First-principles study of the rocksalt□esium chloride relative phase stability in alkali halides. *Physical Review B*, **2002**, 66,	3.3	432
194	Quantum-Mechanical Study of Thermodynamic and Bonding Properties of MgF2. *Journal of Physical Chemistry A*, **1998**, 102, 1595-1601	2.8	374
193	Bond paths as privileged exchange channels. *Chemistry - A European Journal*, **2007**, 13, 9362-71	4.8	260
192	A Molecular Energy Decomposition Scheme for Atoms in Molecules. *Journal of Chemical Theory and Computation*, **2006**, 2, 90-102	6.4	232
191	Critic: a new program for the topological analysis of solid-state electron densities. *Computer Physics Communications*, **2009**, 180, 157-166	4.2	231
190	The nature of the hydrogen bond: a synthesis from the interacting quantum atoms picture. *Journal of Chemical Physics*, **2006**, 125, 184112	3.9	183
189	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
188	Two-electron integrations in the quantum theory of atoms in molecules. *Journal of Chemical Physics* , **2004**, 120, 4581-92	3.9	143
187	Non-nuclear Maxima of the Electron Density. *Physical Review Letters*, **1999**, 83, 1930-1933	7.4	137
186	Chemical fragments in real space: definitions, properties, and energetic decompositions. *Journal of Computational Chemistry*, **2007**, 28, 161-84	3.5	119
185	Local compressibilities in crystals. *Physical Review B*, **2000**, 62, 13970-13978	3.3	118
184	Ions in crystals: The topology of the electron density in ionic materials. I. Fundamentals. *Physical Review B*, **1997**, 55, 4275-4284	3.3	111
183	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
182	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
181	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

180	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
179	Theoretical explanation of the uniform compressibility behavior observed in oxide spinels. *Physical Review B*, **2001**, 63,	3.3	88
178	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
177	Hydrogen bond cooperativity and anticooperativity within the water hexamer. *Physical Chemistry Chemical Physics*, **2016**, 18, 19557-66	3.6	83
176	Six questions on topology in theoretical chemistry. *Computational and Theoretical Chemistry*, **2015**, 1053, 2-16	2	81
175	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
174	Pressure-induced B1-B2 phase transition in alkali halides: General aspects from first-principles calculations. *Physical Review B*, **1994**, 49, 3066-3074	3.3	78
173	Revitalizing the concept of bond order through delocalization measures in real space. *Chemical Science*, **2018**, 9, 5517-5529	9.4	77
172	Domain-averaged exchange-correlation energies as a physical underpinning for chemical graphs. *ChemPhysChem*, **2013**, 14, 1211-8	3.2	74
171	Steric repulsions, rotation barriers, and stereoelectronic effects: a real space perspective. *Journal of Computational Chemistry*, **2009**, 30, 98-109	3.5	74
170	Rigorous characterization of oxygen vacancies in ionic oxides. *Physical Review B*, **2002**, 66,	3.3	72
169	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
168	Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, **2019**, 40, 2248-2283	3.5	70
167	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
166	Electron number probability distributions for correlated wave functions. *Journal of Chemical Physics* , **2007**, 126, 094102	3.9	66
165	Chemical bonding in group III nitrides. *Journal of the American Chemical Society*, **2002**, 124, 4116-23	16.4	66
164	Quantum-mechanical analysis of the equation of state of anatase TiO2. *Physical Review B*, **2001**, 64,	3.3	63
163	An electron number distribution view of chemical bonds in real space. *Physical Chemistry Chemical Physics*, **2007**, 9, 1087-92	3.6	57

162	Topological Analysis of Chemical Bonding in Cyclophosphazenes. *Journal of Physical Chemistry A*, **2001**, 105, 5280-5291	2.8	53
161	Dative and Electron-Sharing Bonding in C F. *Chemistry - A European Journal*, **2018**, 24, 9083-9089	4.8	50
160	Generalized Huzinaga building-block equations for nonorthogonal electronic groups: Relation to the Adams□Gilbert theory. *Journal of Chemical Physics*, **1992**, 97, 6504-6508	3.9	50
159	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
158	Nature of Chemical Interactions from the Profiles of Electron Delocalization Indices. *Journal of Chemical Theory and Computation*, **2011**, 7, 1704-11	6.4	48
157	The nature of resonance-assisted hydrogen bonds: a quantum chemical topology perspective. *Physical Chemistry Chemical Physics*, **2016**, 18, 26383-90	3.6	48
156	Non-nuclear maxima of the electron density on alkaline metals. *Journal of Chemical Physics*, **2003**, 119, 6341-6350	3.9	47
155	Spin resolved electron number distribution functions: how spins couple in real space. *Journal of Chemical Physics*, **2007**, 127, 144103	3.9	46
154	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
153	Stress, virial, and pressure in the theory of atoms in molecules. *Journal of Chemical Physics*, **2002**, 117, 965-979	3.9	44
152	Quantum mechanical cluster calculations of ionic materials: the ab initio perturbed ion (version 7) program. *Computer Physics Communications*, **1993**, 77, 107-134	4.2	42
151	Bond metallicity of materials from real space charge density distributions. *Chemical Physics Letters*, **2009**, 471, 174-177	2.5	41
150	Low- and high-pressure ab initio equations of state for the alkali chlorides. *Physical Review B*, **1993**, 48, 5891-5901	3.3	41
149	EDF: Computing electron number probability distribution functions in real space from molecular wave functions. *Computer Physics Communications*, **2008**, 178, 621-634	4.2	40
148	Pauling resonant structures in real space through electron number probability distributions. *Journal of Physical Chemistry A*, **2007**, 111, 1084-90	2.8	40
147	Evolution of the properties of Al(n)N(n) clusters with size. *Journal of Physical Chemistry B*, **2005**, 109, 24352-60	3.4	39
146	Partitioning the DFT exchange-correlation energy in line with the interacting quantum atoms approach. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	37
145	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

144	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
143	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
142	Dynamical correlation within the Interacting Quantum Atoms method through coupled cluster theory. *Computational and Theoretical Chemistry*, **2015**, 1053, 90-95	2	33
141	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
140	A multipolar approach to the interatomic covalent interaction energy. *Journal of Computational Chemistry*, **2017**, 38, 816-829	3.5	32
139	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
138	Hirshfeld surfaces as approximations to interatomic surfaces. *Journal of Chemical Physics*, **2002**, 117, 1017-1023	3.9	31
137	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
136	Unusual substituent effects on the bonding of iminoboranes. *Physical Chemistry Chemical Physics*, **2007**, 9, 3970-7	3.6	29
135	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
134	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
133	Understanding the bifurcated halogen bonding N?Hal?N in bidentate diazaheterocyclic compounds. *Computational and Theoretical Chemistry*, **2015**, 1053, 229-237	2	27
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131	Interacting Quantum Atoms-A Review. *Molecules*, **2020**, 25,	4.8	27
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127	Electron correlation in the interacting quantum atoms partition via coupled-cluster lagrangian densities. *Journal of Computational Chemistry*, **2016**, 37, 1753-65	3.5	26

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125	One-electron images in real space: natural adaptive orbitals. *Journal of Computational Chemistry*, **2015**, 36, 833-43	3.5	25
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123	Static simulations of CaF2 polymorphs. *Physical Review B*, **1994**, 49, 5858-5868	3.3	25
122	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
121	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
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118	Derivation of electron-gas interatomic potentials from quantum-mechanical descriptions of ions in crystals. *Physical Review B*, **1995**, 51, 2703-2714	3.3	23
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116	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
115	A view of covalent and ionic bonding from Maximum Probability Domains. *Computational and Theoretical Chemistry*, **2015**, 1053, 142-149	2	21
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111	Where Does Electron Correlation Lie? Some Answers from a Real Space Partition. *ChemPhysChem*, **2017**, 18, 3553-3561	3.2	19
110	An anatomy of intramolecular atomic interactions in halogen-substituted trinitromethanes. *Physical Chemistry Chemical Physics*, **2014**, 16, 16780-9	3.6	19
109	Spatial localization, correlation, and statistical dependence of electrons in atomic domains: The . *Chemical Physics Letters*, **2007**, 437, 287-292	2.5	19

108	The bifunctional catalytic role of water clusters in the formation of acid rain. *Chemical Communications*, **2017**, 53, 3516-3519	5.8	18
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102	Hydrogen-Bond Weakening through □ Systems: Resonance-Impaired Hydrogen Bonds (RIHB). *Chemistry - A European Journal*, **2017**, 23, 16605-16611	4.8	17
101	Revisiting the variational nature of the quantum theory of atoms in molecules. *Chemical Physics Letters*, **2006**, 417, 16-21	2.5	17
100	Fermi and Coulomb correlation effects upon the interacting quantum atoms energy partition. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	17
99	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
98	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
97	Microscopic analysis of the compressibility in the spinel phase of Si 3 N 4. *Europhysics Letters*, **2001**, 54, 760-766	1.6	16
96	Real space bond orders are energetic descriptors. *Physical Chemistry Chemical Physics*, **2018**, 20, 16231-16237	3.3	16
95	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
94	Comparison of direct and flow integration based charge density population analyses. *Journal of Physical Chemistry A*, **2007**, 111, 12146-51	2.8	15
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91	Beryllium Bonding in the Light of Modern Quantum Chemical Topology Tools. *Journal of Physical Chemistry A*, **2018**, 122, 849-858	2.8	14

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88	Bases for Understanding Polymerization under Pressure: The Practical Case of CO2. *Journal of Physical Chemistry B*, **2009**, 113, 1068-73	3.4	13
87	Overlap, effective-potential, and projection-operator bicentric integrals over complex Slater-type orbitals. *Physical Review A*, **1991**, 43, 3384-3391	2.6	13
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85	Generalized electron number distribution functions: real space versus orbital space descriptions. *Theoretical Chemistry Accounts*, **2011**, 128, 433-444	1.9	12
84	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
83	On the strength of hydrogen bonding within water clusters on the coordination limit. *Journal of Computational Chemistry*, **2020**, 41, 2266-2277	3.5	12
82	Partition of electronic excitation energies: the IQA/EOM-CCSD method. *Physical Chemistry Chemical Physics*, **2019**, 21, 13428-13439	3.6	11
81	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
80	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
79	Ab initio pair potentials from quantum-mechanical atoms-in-crystals calculations. *Journal of Physics Condensed Matter*, **1993**, 5, 4975-4988	1.8	11
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68	How Electronic Excitation Can be Used to Inhibit Some Mechanisms Associated to Substituent Effects. *ChemPhysChem*, **2016**, 17, 2666-71	3.2	8
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66	Electron number distribution functions with iterative Hirshfeld atoms. *Computational and Theoretical Chemistry*, **2011**, 975, 2-8	2	8
65	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
64	Laplacian of the Hamiltonian Kinetic Energy Density as an Indicator of Binding and Weak Interactions. *ChemPhysChem*, **2020**, 21, 194-203	3.2	8
63	Bond Order Densities in Real Space. *Journal of Physical Chemistry A*, **2020**, 124, 339-352	2.8	8
62	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
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60	Tetrel Interactions from an Interacting Quantum Atoms Perspective. *Molecules*, **2019**, 24,	4.8	7
59	Structural effects of trifluoromethylation and fluorination in gold(I) BIPHEP fluorothiolates. *New Journal of Chemistry*, **2017**, 41, 10537-10541	3.6	7
58	Efficient algorithms for Hirshfeld-I charges. *Journal of Chemical Physics*, **2015**, 143, 084115	3.9	7
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55	Ionic properties of perovskites derived from topological analysis of their wave function. *Journal of Physics Condensed Matter*, **1999**, 11, 6329-6336	1.8	7

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47	Curvature of interatomic surfaces. I. Fundamentals. *Journal of Chemical Physics*, **2003**, 119, 7633-7642	3.9	6
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45	Performance of the RI and RIJCOSX approximations in the topological analysis of the electron density. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	5
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27	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
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