Evelio E Francisco MiguÃ©lez

List of Publications by Year
in descending order

138 papers	7,991 citations	94269 37 h-index	49773 87 g-index
144 all docs	144 docs citations	144 times ranked	3071 citing authors

#	Article	IF	Citations
1	GIBBS: isothermal-isobaric thermodynamics of solids from energy curves using a quasi-harmonic Debye model. Computer Physics Communications, 2004, 158, 57-72.	3.0	1,598
2	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
3	Thermodynamical properties of solids from microscopic theory: applications to MgF2 and Al2O3. Computational and Theoretical Chemistry, 1996, 368, 245-255.	1.5	523
4	First-principles study of the rocksaltâ€“cesium chloride relative phase stability in alkali halides. Physical Review B, 2002, 66, .	1.1	484
5	Atomistic simulation ofSrF2polymorphs. Physical Review B, 2001, 63, .	1.1	475
6	Quantum-Mechanical Study of Thermodynamic and Bonding Properties of MgF2. Journal of Physical Chemistry A, 1998, 102, 1595-1601.	1.1	410
7	Bond Paths as Privileged Exchange Channels. Chemistry - A European Journal, 2007, 13, 9362-9371.	1.7	297
8	A Molecular Energy Decomposition Scheme for Atoms in Molecules. Journal of Chemical Theory and Computation, 2006, 2, 90-102.	2.3	271
9	The nature of the hydrogen bond: A synthesis from the interacting quantum atoms picture. Journal of Chemical Physics, 2006, 125, 184112.	1.2	208
10	Two-electron integrations in the quantum theory of atoms in molecules. Journal of Chemical Physics, 2004, 120, 4581-4592.	1.2	157
11	Chemical fragments in real space: Definitions, properties, and energetic decompositions. Journal of Computational Chemistry, 2007, 28, 161-184.	1.5	138
12	Hydrogen bond cooperativity and anticooperativity within the water hexamer. Physical Chemistry Chemical Physics, 2016, 18, 19557-19566.	1.3	106
13	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
14	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
15	Domainâ€Averaged Exchangeâ€Correlation Energies as a Physical Underpinning for Chemical Graphs. ChemPhysChem, 2013, 14, 1211-1218.	1.0	89
16	Pressure-inducedB1-B2 phase transition in alkali halides: General aspects from first-principles calculations. Physical Review B, 1994, 49, 3066-3074.	1.1	82
17	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
18	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

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19	Steric repulsions, rotation barriers, and stereoelectronic effects: A real space perspective. Journal of Computational Chemistry, 2009, 30, 98-109.	1.5	78
20	Electron number probability distributions for correlated wave functions. Journal of Chemical Physics, 2007, 126, 094102.	1.2	69
21	Quantum-mechanical analysis of the equation of state of anataseTiO2. Physical Review B, 2001, 64, .	1.1	68
22	Interacting Quantum Atomsâ€"A Review. Molecules, 2020, 25, 4028.	1.7	67
23	An electron number distribution view of chemical bonds in real space. Physical Chemistry Chemical Physics, 2007, 9, 1087-1092.	1.3	59
24	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
25	Nature of Chemical Interactions from the Profiles of Electron Delocalization Indices. Journal of Chemical Theory and Computation, 2011, 7, 1704-1711.	2.3	51
26	Partitioning the DFT exchange-correlation energy in line with the interacting quantum atoms approach. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	50
27	Low- and high-pressureab initioequations of state for the alkali chlorides. Physical Review B, 1993, 48, 5891-5901.	1.1	47
28	Spin resolved electron number distribution functions: How spins couple in real space. Journal of Chemical Physics, 2007, 127, 144103.	1.2	47
29	Oneâ€electron images in real space: Natural adaptive orbitals. Journal of Computational Chemistry, 2015, 36, 833-843.	1.5	46
30	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
31	Pauling Resonant Structures in Real Space through Electron Number Probability Distributions. Journal of Physical Chemistry A, 2007, 111, 1084-1090.	1.1	43
32	EDF: Computing electron number probability distribution functions in real space from molecular wave functions. Computer Physics Communications, 2008, 178, 621-634.	3.0	43
33	Hirshfeld surfaces as approximations to interatomic surfaces. Journal of Chemical Physics, 2002, 117, 1017-1023.	1.2	41
34	Evolution of the Properties of AlnNnClusters with Size. Journal of Physical Chemistry B, 2005, 109, 24352-24360.	1.2	40
35	Charge transfer, chemical potentials, and the nature of functional groups: answers from quantum chemical topology. Faraday Discussions, 2007, 135, 423-438.	1.6	40
36	A multipolar approach to the interatomic covalent interaction energy. Journal of Computational Chemistry, 2017, 38, 816-829.	1.5	40

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37	Dynamical correlation within the Interacting Quantum Atoms method through coupled cluster theory. Computational and Theoretical Chemistry, 2015, 1053, 90-95.	1.1	39
38	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
39	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
40	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
41	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
42	Electron correlation in the interacting quantum atoms partition via coupledâ€cluster lagrangian densities. Journal of Computational Chemistry, 2016, 37, 1753-1765.	1.5	32
43	Bond Order Densities in Real Space. Journal of Physical Chemistry A, 2020, 124, 339-352.	1.1	31
44	Electronâ€“electron interactions between ELF basins. Chemical Physics Letters, 2008, 454, 396-403.	1.2	30
45	On Electrostatics, Covalency, and Chemical Dashes: Physical Interactions versus Chemical Bonds. Chemistry - A European Journal, 2019, 25, 309-314.	1.7	30
46	A Theoretical Study of the Cluster Vibrations in Cr2O2, Cr2O3, and Cr2O4. Journal of Physical Chemistry A, 2000, 104, 990-994.	1.1	29
47	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
48	Using Pseudopotentials within the Interacting Quantum Atoms Approach. Journal of Physical Chemistry A, 2009, 113, 7963-7971.	1.1	24
49	On the interpretation of domain averaged Fermi hole analyses of correlated wavefunctions. Physical Chemistry Chemical Physics, 2014, 16, 4586.	1.3	24
50	Where Does Electron Correlation Lie? Some Answers from a Real Space Partition. ChemPhysChem, 2017, 18, 3553-3561.	1.0	24
51	Derivation of electron-gas interatomic potentials from quantum-mechanical descriptions of ions in crystals. Physical Review B, 1995, 51, 2703-2714.	1.1	23
52	Chemical Bonding from the Statistics of the Electron Distribution. ChemPhysChem, 2019, 20, 2722-2741.	1.0	22
53	Energy Partition Analyses: Symmetry-Adapted Perturbation Theory and Other Techniques. , 2017, , 27-64.		21
54	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

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55	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,	1.2	20
56	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
57	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
58	Beryllium Bonding in the Light of Modern Quantum Chemical Topology Tools. Journal of Physical Chemistry A, 2018, 122, 849-858.	1.1	20
59	Real space bond orders are energetic descriptors. Physical Chemistry Chemical Physics, 2018, 20, 16231-16237.	1.3	20
60	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
61	Revisiting the variational nature of the quantum theory of atoms in molecules. Chemical Physics Letters, 2006, 417, 16-21.	1.2	19
62	Electron number distribution functions from molecular wavefunctions. Version 2. Computer Physics Communications, 2014, 185, 2663-2682.	3.0	19
63	Accurate calculation of spin-orbit coupling constants for 3datoms and ions with effective core potentials and reduced basis sets. Physical Review A, 1987, 36, 1978-1982.	1.0	18
64	Theoretical spin-orbit coupling constants for 3dions in crystals. Physical Review B, 1988, 37, 5278-5288.	1.1	18
65	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
66	Fermi and Coulomb correlation effects upon the interacting quantum atoms energy partition. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	17
67	Partition of electronic excitation energies: the IQA/EOM-CCSD method. Physical Chemistry Chemical Physics, 2019, 21, 13428-13439.	1.3	17
68	The maximum overlap method: A general and efficient scheme for reducing basis sets. Application to the generation of approximate AO's for the 3d transition metal atoms and ions. Journal of Solid State Chemistry, 1986, 63, 391-400.	1.4	16
69	Comparison of Direct and Flow Integration Based Charge Density Population Analyses. Journal of Physical Chemistry A, 2007, 111, 12146-12151.	1.1	16
70	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
71	Quantum Chemical Topology as a Theory of Open Quantum Systems. Journal of Chemical Theory and Computation, 2019, 15, 1079-1088.	2.3	16
72	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

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73	Anti-ohmic single molecule electron transport: is it feasible?. Nanoscale Advances, 2019, 1, 1901-1913.	2.2	15
74	Core projection effects in near-ab-initio valence calculations. Journal of Solid State Chemistry, 1987, 66, 263-282.	1.4	14
75	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
76	Global optimization of ionic MgnF2n (n=1â€“30) clusters. Journal of Chemical Physics, 2005, 123, 234305.	1.2	14
77	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
78	Decoding real space bonding descriptors in valence bond language. Physical Chemistry Chemical Physics, 2018, 20, 12368-12372.	1.3	14
79	Overlap, effective-potential, and projection-operator bicentric integrals over complex Slater-type orbitals. Physical Review A, 1991, 43, 3384-3391.	1.0	13
80	Fluorine conformational effects characterized by energy decomposition analysis. Physical Chemistry Chemical Physics, 2019, 21, 25258-25275.	1.3	13
81	Ab initio pair potentials from quantum-mechanical atoms-in-crystals calculations. Journal of Physics Condensed Matter, 1993, 5, 4975-4988.	0.7	12
82	Generalized electron number distribution functions: real space versus orbital space descriptions. Theoretical Chemistry Accounts, 2011, 128, 433-444.	0.5	12
83	Structure and Bonding in Magnesium Difluoride Clusters:Â The MgF2Molecule. Journal of Physical Chemistry A, 2001, 105, 4126-4135.	1.1	11
84	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
85	Exotic Bonding Regimes Uncovered in Excited States. Chemistry - A European Journal, 2019, 25, 12169-12179.	1.7	10
86	Tetrel Interactions from an Interacting Quantum Atoms Perspective. Molecules, 2019, 24, 2204.	1.7	10
87	Local spin and open quantum systems: clarifying misconceptions, unifying approaches. Physical Chemistry Chemical Physics, 2021, 23, 8375-8392.	1.3	10
88	Atomistic simulation of the pressure-temperature-volume diagram in Î±-Al2O3. Solid State Communications, 1996, 98, 41-44.	0.9	9
89	Spinodal equation of state for rutileTiO2. Physical Review B, 2003, 67, .	1.1	9
90	Efficient algorithms for Hirshfeld-I charges. Journal of Chemical Physics, 2015, 143, 084115.	1.2	9

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91	How Electronic Excitation Can be Used to Inhibit Some Mechanisms Associated to Substituent Effects. ChemPhysChem, 2016, 17, 2666-2671.	1.0	9
92	Electron number distribution functions with iterative Hirshfeld atoms. Computational and Theoretical Chemistry, 2011, 975, 2-8.	1.1	8
93	Emergent Scalar and Vector Fields in Quantum Chemical Topology. Challenges and Advances in Computational Chemistry and Physics, 2016, , 131-150.	0.6	8
94	From quantum fragments to Lewis structures: electron counting in position space. Physical Chemistry Chemical Physics, 2018, 20, 21368-21380.	1.3	8
95	Photochemistry in Real Space: Bathoâ€•and Hypsochromism in the Water Dimer. Chemistry - A European Journal, 2020, 26, 17035-17045.	1.7	8
96	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
97	Modeling theO2â^'-O2â^'interaction for atomistic simulations. Physical Review B, 1995, 51, 11289-11295.	1.1	7
98	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
99	Interacting Quantum Atoms Method for Crystalline Solids. Journal of Physical Chemistry A, 2021, 125, 9011-9025.	1.1	7
100	A new model for the cluster-lattice interaction in cluster-type calculations of transition-metal ions in crystals. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1987, 84, 863-869.	0.2	7
101	Beyond Standard Charge Density Topological Analyses. , 2011, , 303-358.		6
102	Perspectives for quantum chemical topology in crystallography. Physica Scripta, 2013, 87, 048106.	1.2	6
103	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
104	QM/MM Energy Decomposition Using the Interacting Quantum Atoms Approach. Journal of Chemical Information and Modeling, 2022, 62, 1510-1524.	2.5	6
105	The role of references and the elusive nature of the chemical bond. Nature Communications, 2022, 13, .	5.8	6
106	The coulombic lattice potential of ionic compounds: The cubic perovskites. Journal of Chemical Education, 1988, 65, 6.	1.1	5
107	Exact versus truncated spectrally resolved exchange in ab initio calculations. Journal of Chemical Physics, 1992, 97, 452-458.	1.2	5
108	Inference of crystal properties from cluster magnitudes. Journal of Chemical Physics, 1995, 103, 432-439.	1.2	5

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109	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
110	Theoretical Simulation of AlN Nanocrystals. Journal of Physical Chemistry C, 2008, 112, 6667-6676.	1.5	5
111	Interacting Quantum Atoms Approach and Electrostatic Solvation Energy: Assessing Atomic and Group Solvation Contributions. ChemPhysChem, 2018, 19, 3425-3435.	1.0	5
112	Electron-pair bonding in real space. Is the charge-shift family supported?. Chemical Communications, 2019, 55, 5071-5074.	2.2	5
113	Electronegativity equalization: taming an old problem with new tools. Physical Chemistry Chemical Physics, 2020, 22, 22880-22884.	1.3	4
114	3d-4s and 3d-4p electronic transitions in M²⁺ : NaF AND M²⁺ : KMgF³ (Îœ = V, Cr, and Mn). Results of a cluster-model calculation. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1987, 84, 855-861.	0.2	4
115	Implementation of the interacting quantum atom energy decomposition using the CASPT2 method. Physical Chemistry Chemical Physics, 2021, 23, 27508-27519.	1.3	4
116	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
117	Basis sets generation: Relation between Adamowicz's and the maximum overlap method. International Journal of Quantum Chemistry, 1987, 31, 279-285.	1.0	3
118	Strategies for determining and usingab initiointerionic potentials. Radiation Effects and Defects in Solids, 1999, 151, 223-228.	0.4	3
119	Atomistic Simulation of the Equation of State of SrF 2 Using Electron Gas Interionic Potentials. High Pressure Research, 2002, 22, 227-230.	0.4	3
120	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
121	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
122	The nature of the intermolecular interaction in (H2X)2 (X = O, S, Se). Physical Chemistry Chemical Physics, 2021, 23, 10097-10107.	1.3	3
123	Reduction of orbital sets. Computer Physics Communications, 1987, 43, 269-277.	3.0	2
124	DFT performance in the IQA energy partition of small water clusters. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	2
125	Questioning the orbital picture of magnetic spin coupling: a real space alternative. Physical Chemistry Chemical Physics, 2022, 24, 639-652.	1.3	2
126	Energetics of the RbF + CaF2 â†' RbCaF3 solid state reaction: A first-principles study. Radiation Effects and Defects in Solids, 1995, 134, 193-196.	0.4	1

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127	Theoretical study of the coordination of the Cr³⁺ ion in Î±-Al₂O₃. Radiation Effects and Defects in Solids, 1995, 134, 123-126.	0.4	1
128	Microscopic Study of the Rock Salt-Caesium Chloride Phase Stability in Alkali Halides. High Pressure Research, 2002, 22, 443-446.	0.4	1
129	An energy partition method based on localized molecular orbitals. Computational and Theoretical Chemistry, 2015, 1053, 77-84.	1.1	1
130	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
131	Localization and Delocalization in Solids from Electron Distribution Functions. Journal of Chemical Theory and Computation, 0, , .	2.3	1
132	Local wave functions for multinegative ions in solids. Radiation Effects and Defects in Solids, 1991, 119-121, 727-728.	0.4	0
133	Theoretical computation of the gyromagnetic factor for the Cr³⁺and V²⁺ions in KMgF₃. Radiation Effects and Defects in Solids, 1991, 119-121, 725-726.	0.4	0
134	Theoretical d-d spectrum of Cr3+:Mg0. Radiation Effects and Defects in Solids, 1991, 119-121, 437-438.	0.4	0
135	Stability of B1 and B2 phases from electronic density topology considerations. Radiation Effects and Defects in Solids, 1995, 134, 201-203.	0.4	0
136	Effects of a quantum crystal potential on the derivation of electron gas interionic energies. Radiation Effects and Defects in Solids, 1995, 134, 197-200.	0.4	0
137	Reduced-size representations of high-quality atomic densities. The hybrid Gaussian?exponential case. Theoretical Chemistry Accounts, 2004, 112, 113.	0.5	0
138	Photochemistry in Real Space: Bathoâ€•and Hypsochromism in the Water Dimer. Chemistry - A European Journal, 2020, 26, 16951-16951.	1.7	0