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	Questioning the orbital picture of magnetic spin coupling: a real space alternative. Physical Chemistry Chemical Physics, 2022, 24, 639-652.	1.3	2
2	QM/MM Energy Decomposition Using the Interacting Quantum Atoms Approach. Journal of Chemical Information and Modeling, 2022, 62, 1510-1524.	2.5	6
3	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
4	The role of references and the elusive nature of the chemical bond. Nature Communications, 2022, 13, .	5.8	6
5	The nature of the intermolecular interaction in (H2X)2 (X = O, S, Se). Physical Chemistry Chemical Physics, 2021, 23, 10097-10107.	1.3	3
6	Local spin and open quantum systems: clarifying misconceptions, unifying approaches. Physical Chemistry Chemical Physics, 2021, 23, 8375-8392.	1.3	10
7	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
8	Interacting Quantum Atoms Method for Crystalline Solids. Journal of Physical Chemistry A, 2021, 125, 9011-9025.	1.1	7
9	Implementation of the interacting quantum atom energy decomposition using the CASPT2 method. Physical Chemistry Chemical Physics, 2021, 23, 27508-27519.	1.3	4
10	Bond Order Densities in Real Space. Journal of Physical Chemistry A, 2020, 124, 339-352.	1.1	31
11	DFT performance in the IQA energy partition of small water clusters. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	2
12	Electronegativity equalization: taming an old problem with new tools. Physical Chemistry Chemical Physics, 2020, 22, 22880-22884.	1.3	4
13	Interacting Quantum Atomsâ€”A Review. Molecules, 2020, 25, 4028.	1.7	67
14	Photochemistry in Real Space: Bathoâ€•and Hypsochromism in the Water Dimer. Chemistry - A European Journal, 2020, 26, 17035-17045.	1.7	8
15	Photochemistry in Real Space: Bathoâ€•and Hypsochromism in the Water Dimer. Chemistry - A European Journal, 2020, 26, 16951-16951.	1.7	0
16	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
17	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
18	Exotic Bonding Regimes Uncovered in Excited States. Chemistry - A European Journal, 2019, 25, 12169-12179.	1.7	10

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19	Tetrel Interactions from an Interacting Quantum Atoms Perspective. Molecules, 2019, 24, 2204.	1.7	10
20	Chemical Bonding from the Statistics of the Electron Distribution. ChemPhysChem, 2019, 20, 2722-2741.	1.0	22
21	Partition of electronic excitation energies: the IQA/EOM-CCSD method. Physical Chemistry Chemical Physics, 2019, 21, 13428-13439.	1.3	17
22	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
23	Anti-ohmic single molecule electron transport: is it feasible?. Nanoscale Advances, 2019, 1, 1901-1913.	2.2	15
24	Electron-pair bonding in real space. Is the charge-shift family supported?. Chemical Communications, 2019, 55, 5071-5074.	2.2	5
25	Fluorine conformational effects characterized by energy decomposition analysis. Physical Chemistry Chemical Physics, 2019, 21, 25258-25275.	1.3	13
26	Quantum Chemical Topology as a Theory of Open Quantum Systems. Journal of Chemical Theory and Computation, 2019, 15, 1079-1088.	2.3	16
27	On Electrostatics, Covalency, and Chemical Dashes: Physical Interactions versus Chemical Bonds. Chemistry - A European Journal, 2019, 25, 309-314.	1.7	30
28	Decoding real space bonding descriptors in valence bond language. Physical Chemistry Chemical Physics, 2018, 20, 12368-12372.	1.3	14
29	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
30	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
31	Beryllium Bonding in the Light of Modern Quantum Chemical Topology Tools. Journal of Physical Chemistry A, 2018, 122, 849-858.	1.1	20
32	Interacting Quantum Atoms Approach and Electrostatic Solvation Energy: Assessing Atomic and Group Solvation Contributions. ChemPhysChem, 2018, 19, 3425-3435.	1.0	5
33	Real space bond orders are energetic descriptors. Physical Chemistry Chemical Physics, 2018, 20, 16231-16237.	1.3	20
34	From quantum fragments to Lewis structures: electron counting in position space. Physical Chemistry Chemical Physics, 2018, 20, 21368-21380.	1.3	8
35	A multipolar approach to the interatomic covalent interaction energy. Journal of Computational Chemistry, 2017, 38, 816-829.	1.5	40
36	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

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37	Where Does Electron Correlation Lie? Some Answers from a Real Space Partition. ChemPhysChem, 2017, 18, 3553-3561.	1.0	24
38	Energy Partition Analyses: Symmetry-Adapted Perturbation Theory and Other Techniques. , 2017, , 27-64.		21
39	Partitioning the DFT exchange-correlation energy in line with the interacting quantum atoms approach. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	50
40	Electron correlation in the interacting quantum atoms partition via coupledâ€cluster lagrangian densities. Journal of Computational Chemistry, 2016, 37, 1753-1765.	1.5	32
41	Hydrogen bond cooperativity and anticooperativity within the water hexamer. Physical Chemistry Chemical Physics, 2016, 18, 19557-19566.	1.3	106
42	Emergent Scalar and Vector Fields in Quantum Chemical Topology. Challenges and Advances in Computational Chemistry and Physics, 2016, , 131-150.	0.6	8
43	Fermi and Coulomb correlation effects upon the interacting quantum atoms energy partition. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	17
44	How Electronic Excitation Can be Used to Inhibit Some Mechanisms Associated to Substituent Effects. ChemPhysChem, 2016, 17, 2666-2671.	1.0	9
45	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
46	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
47	Efficient algorithms for Hirshfeld-I charges. Journal of Chemical Physics, 2015, 143, 084115.	1.2	9
48	Oneâ€electron images in real space: Natural adaptive orbitals. Journal of Computational Chemistry, 2015, 36, 833-843.	1.5	46
49	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
50	An energy partition method based on localized molecular orbitals. Computational and Theoretical Chemistry, 2015, 1053, 77-84.	1.1	1
51	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
52	Dynamical correlation within the Interacting Quantum Atoms method through coupled cluster theory. Computational and Theoretical Chemistry, 2015, 1053, 90-95.	1.1	39
53	On the interpretation of domain averaged Fermi hole analyses of correlated wavefunctions. Physical Chemistry Chemical Physics, 2014, 16, 4586.	1.3	24
54	Electron number distribution functions from molecular wavefunctions. Version 2. Computer Physics Communications, 2014, 185, 2663-2682.	3.0	19

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55	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
56	Perspectives for quantum chemical topology in crystallography. Physica Scripta, 2013, 87, 048106.	1.2	6
57	Domainâ€Averaged Exchangeâ€Correlation Energies as a Physical Underpinning for Chemical Graphs. ChemPhysChem, 2013, 14, 1211-1218.	1.0	89
58	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
59	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
60	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
61	Beyond Standard Charge Density Topological Analyses. , 2011, , 303-358.		6
62	Nature of Chemical Interactions from the Profiles of Electron Delocalization Indices. Journal of Chemical Theory and Computation, 2011, 7, 1704-1711.	2.3	51
63	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
64	Electron number distribution functions with iterative Hirshfeld atoms. Computational and Theoretical Chemistry, 2011, 975, 2-8.	1.1	8
65	Generalized electron number distribution functions: real space versus orbital space descriptions. Theoretical Chemistry Accounts, 2011, 128, 433-444.	0.5	12
66	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
67	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
68	Steric repulsions, rotation barriers, and stereoelectronic effects: A real space perspective. Journal of Computational Chemistry, 2009, 30, 98-109.	1.5	78
69	Using Pseudopotentials within the Interacting Quantum Atoms Approach. Journal of Physical Chemistry A, 2009, 113, 7963-7971.	1.1	24
70	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
71	EDF: Computing electron number probability distribution functions in real space from molecular wave functions. Computer Physics Communications, 2008, 178, 621-634.	3.0	43
72	Electronâ€“electron interactions between ELF basins. Chemical Physics Letters, 2008, 454, 396-403.	1.2	30

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73	Theoretical Simulation of AlN Nanocrystals. Journal of Physical Chemistry C, 2008, 112, 6667-6676.	1.5	5
74	Pauling Resonant Structures in Real Space through Electron Number Probability Distributions. Journal of Physical Chemistry A, 2007, 111, 1084-1090.	1.1	43
75	An electron number distribution view of chemical bonds in real space. Physical Chemistry Chemical Physics, 2007, 9, 1087-1092.	1.3	59
76	Comparison of Direct and Flow Integration Based Charge Density Population Analyses. Journal of Physical Chemistry A, 2007, 111, 12146-12151.	1.1	16
77	Spin resolved electron number distribution functions: How spins couple in real space. Journal of Chemical Physics, 2007, 127, 144103.	1.2	47
78	Charge transfer, chemical potentials, and the nature of functional groups: answers from quantum chemical topology. Faraday Discussions, 2007, 135, 423-438.	1.6	40
79	Bond Paths as Privileged Exchange Channels. Chemistry - A European Journal, 2007, 13, 9362-9371.	1.7	297
80	Chemical fragments in real space: Definitions, properties, and energetic decompositions. Journal of Computational Chemistry, 2007, 28, 161-184.	1.5	138
81	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
82	Electron number probability distributions for correlated wave functions. Journal of Chemical Physics, 2007, 126, 094102.	1.2	69
83	A Molecular Energy Decomposition Scheme for Atoms in Molecules. Journal of Chemical Theory and Computation, 2006, 2, 90-102.	2.3	271
84	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
85	The nature of the hydrogen bond: A synthesis from the interacting quantum atoms picture. Journal of Chemical Physics, 2006, 125, 184112.	1.2	208
86	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
87	Revisiting the variational nature of the quantum theory of atoms in molecules. Chemical Physics Letters, 2006, 417, 16-21.	1.2	19
88	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
89	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
90	Global optimization of ionic MgnF2n (n=1â€“30) clusters. Journal of Chemical Physics, 2005, 123, 234305.	1.2	14

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91	Evolution of the Properties of AlnNnClusters with Size. Journal of Physical Chemistry B, 2005, 109, 24352-24360.	1.2	40
92	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
93	Reduced-size representations of high-quality atomic densities. The hybrid Gaussian?exponential case. Theoretical Chemistry Accounts, 2004, 112, 113.	0.5	0
94	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
95	Two-electron integrations in the quantum theory of atoms in molecules. Journal of Chemical Physics, 2004, 120, 4581-4592.	1.2	157
96	Spinodal equation of state for rutileTiO2. Physical Review B, 2003, 67, .	1.1	9
97	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
98	First-principles study of the rocksaltâ€“cesium chloride relative phase stability in alkali halides. Physical Review B, 2002, 66, .	1.1	484
99	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
100	Microscopic Study of the Rock Salt-Caesium Chloride Phase Stability in Alkali Halides. High Pressure Research, 2002, 22, 443-446.	0.4	1
101	Hirshfeld surfaces as approximations to interatomic surfaces. Journal of Chemical Physics, 2002, 117, 1017-1023.	1.2	41
102	Quantum-mechanical analysis of the equation of state of anataseTiO2. Physical Review B, 2001, 64, .	1.1	68
103	Atomistic simulation ofSrF2polymorphs. Physical Review B, 2001, 63, .	1.1	475
104	Structure and Bonding in Magnesium Difluoride Clusters:Â The MgF2Molecule. Journal of Physical Chemistry A, 2001, 105, 4126-4135.	1.1	11
105	A Theoretical Study of the Cluster Vibrations in Cr2O2, Cr2O3, and Cr2O4. Journal of Physical Chemistry A, 2000, 104, 990-994.	1.1	29
106	Strategies for determining and usingab initiointerionic potentials. Radiation Effects and Defects in Solids, 1999, 151, 223-228.	0.4	3
107	Quantum-Mechanical Study of Thermodynamic and Bonding Properties of MgF2. Journal of Physical Chemistry A, 1998, 102, 1595-1601.	1.1	410
108	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

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109	Thermodynamical properties of solids from microscopic theory: applications to MgF2 and Al2O3. Computational and Theoretical Chemistry, 1996, 368, 245-255.	1.5	523
110	Atomistic simulation of the pressure-temperature-volume diagram in Î±-Al2O3. Solid State Communications, 1996, 98, 41-44.	0.9	9
111	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
112	Inference of crystal properties from cluster magnitudes. Journal of Chemical Physics, 1995, 103, 432-439.	1.2	5
113	Modeling theO2â^'-O2â^'interaction for atomistic simulations. Physical Review B, 1995, 51, 11289-11295.	1.1	7
114	Stability of B1 and B2 phases from electronic density topology considerations. Radiation Effects and Defects in Solids, 1995, 134, 201-203.	0.4	0
115	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
116	Derivation of electron-gas interatomic potentials from quantum-mechanical descriptions of ions in crystals. Physical Review B, 1995, 51, 2703-2714.	1.1	23
117	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
118	Pressure-inducedB1-B2 phase transition in alkali halides: General aspects from first-principles calculations. Physical Review B, 1994, 49, 3066-3074.	1.1	82
119	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
120	Ab initio pair potentials from quantum-mechanical atoms-in-crystals calculations. Journal of Physics Condensed Matter, 1993, 5, 4975-4988.	0.7	12
121	Low- and high-pressureab initioequations of state for the alkali chlorides. Physical Review B, 1993, 48, 5891-5901.	1.1	47
122	Exact versus truncated spectrally resolved exchange in ab initio calculations. Journal of Chemical Physics, 1992, 97, 452-458.	1.2	5
123	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
124	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
125	Local wave functions for multinegative ions in solids. Radiation Effects and Defects in Solids, 1991, 119-121, 727-728.	0.4	0
126	Overlap, effective-potential, and projection-operator bicentric integrals over complex Slater-type orbitals. Physical Review A, 1991, 43, 3384-3391.	1.0	13

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127	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
128	Theoretical d-d spectrum of Cr3+:Mg0. Radiation Effects and Defects in Solids, 1991, 119-121, 437-438.	0.4	0
129	Theoretical spin-orbit coupling constants for 3dions in crystals. Physical Review B, 1988, 37, 5278-5288.	1.1	18
130	The coulombic lattice potential of ionic compounds: The cubic perovskites. Journal of Chemical Education, 1988, 65, 6.	1.1	5
131	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
132	Reduction of orbital sets. Computer Physics Communications, 1987, 43, 269-277.	3.0	2
133	Basis sets generation: Relation between Adamowicz's and the maximum overlap method. International Journal of Quantum Chemistry, 1987, 31, 279-285.	1.0	3
134	Core projection effects in near-ab-initio valence calculations. Journal of Solid State Chemistry, 1987, 66, 263-282.	1.4	14
135	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
136	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
137	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
138	Localization and Delocalization in Solids from Electron Distribution Functions. Journal of Chemical Theory and Computation, 0, , .	2.3	1