Evelio E Francisco Migulez

List of Publications by Year in Descending Order

135 papers	6,804 citations	34 h-index	81 g-index
144 ext. papers	7,358 ext. citations	3.3 avg, IF	5.9 L-index

#	Paper	IF	Citations
135	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
134	The role of references and the elusive nature of the chemical bond. *Nature Communications*, **2022**, 13,	17.4	2
133	Implementation of the interacting quantum atom energy decomposition using the CASPT2 method. *Physical Chemistry Chemical Physics*, **2021**,	3.6	1
132	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
131	The nature of the intermolecular interaction in (HX) (X = O, S, Se). *Physical Chemistry Chemical Physics*, **2021**, 23, 10097-10107	3.6	2
130	Local spin and open quantum systems: clarifying misconceptions, unifying approaches. *Physical Chemistry Chemical Physics*, **2021**, 23, 8375-8392	3.6	5
129	Interacting Quantum Atoms Method for Crystalline Solids. *Journal of Physical Chemistry A*, **2021**, 125, 9011-9025	2.8	2
128	Photochemistry in Real Space: Batho- and Hypsochromism in the Water Dimer. *Chemistry - A European Journal*, **2020**, 26, 16951	4.8	
127	Efficient implementation of the interacting quantum atoms energy partition of the second-order MÏller-Plesset energy. *Journal of Computational Chemistry*, **2020**, 41, 1234-1241	3.5	7
126	Bond Order Densities in Real Space. *Journal of Physical Chemistry A*, **2020**, 124, 339-352	2.8	8
125	DFT performance in the IQA energy partition of small water clusters. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	2
124	Electronegativity equalization: taming an old problem with new tools. *Physical Chemistry Chemical Physics*, **2020**, 22, 22880-22884	3.6	2
123	Interacting Quantum Atoms-A Review. *Molecules*, **2020**, 25,	4.8	27
122	Photochemistry in Real Space: Batho- and Hypsochromism in the Water Dimer. *Chemistry - A European Journal*, **2020**, 26, 17035-17045	4.8	6
121	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
120	Partition of electronic excitation energies: the IQA/EOM-CCSD method. *Physical Chemistry Chemical Physics*, **2019**, 21, 13428-13439	3.6	11
119	Reply to the ŒComment on "Decoding real space bonding descriptors in valence bond language"Œby 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	

118	Anti-ohmic single molecule electron transport: is it feasible?. *Nanoscale Advances*, **2019**, 1, 1901-1913	5.1	10
117	Electron-pair bonding in real space. Is the charge-shift family supported?. *Chemical Communications*, **2019**, 55, 5071-5074	5.8	5
116	Exotic Bonding Regimes Uncovered in Excited States. *Chemistry - A European Journal*, **2019**, 25, 12169-12179	4.8	9
115	Tetrel Interactions from an Interacting Quantum Atoms Perspective. *Molecules*, **2019**, 24,	4.8	7
114	Chemical Bonding from the Statistics of the Electron Distribution. *ChemPhysChem*, **2019**, 20, 2722-2741	3.2	17
113	Fluorine conformational effects characterized by energy decomposition analysis. *Physical Chemistry Chemical Physics*, **2019**, 21, 25258-25275	3.6	7
112	Quantum Chemical Topology as a Theory of Open Quantum Systems. *Journal of Chemical Theory and Computation*, **2019**, 15, 1079-1088	6.4	11
111	On Electrostatics, Covalency, and Chemical Dashes: Physical Interactions versus Chemical Bonds. *Chemistry - A European Journal*, **2019**, 25, 309-314	4.8	21
110	Decoding real space bonding descriptors in valence bond language. *Physical Chemistry Chemical Physics*, **2018**, 20, 12368-12372	3.6	10
109	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
108	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
107	Beryllium Bonding in the Light of Modern Quantum Chemical Topology Tools. *Journal of Physical Chemistry A*, **2018**, 122, 849-858	2.8	14
106	From quantum fragments to Lewis structures: electron counting in position space. *Physical Chemistry Chemical Physics*, **2018**, 20, 21368-21380	3.6	8
105	Interacting Quantum Atoms Approach and Electrostatic Solvation Energy: Assessing Atomic and Group Solvation Contributions. *ChemPhysChem*, **2018**, 19, 3425-3435	3.2	3
104	Real space bond orders are energetic descriptors. *Physical Chemistry Chemical Physics*, **2018**, 20, 16231-16237	3.6	16
103	A multipolar approach to the interatomic covalent interaction energy. *Journal of Computational Chemistry*, **2017**, 38, 816-829	3.5	32
102	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
101	Where Does Electron Correlation Lie? Some Answers from a Real Space Partition. *ChemPhysChem*, **2017**, 18, 3553-3561	3.2	19

100	Energy Partition Analyses: Symmetry-Adapted Perturbation Theory and Other Techniques **2017**, 27-64		13
99	How Electronic Excitation Can be Used to Inhibit Some Mechanisms Associated to Substituent Effects. *ChemPhysChem*, **2016**, 17, 2666-71	3.2	8
98	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
97	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
96	Partitioning the DFT exchange-correlation energy in line with the interacting quantum atoms approach. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	37
95	Electron correlation in the interacting quantum atoms partition via coupled-cluster lagrangian densities. *Journal of Computational Chemistry*, **2016**, 37, 1753-65	3.5	26
94	Hydrogen bond cooperativity and anticooperativity within the water hexamer. *Physical Chemistry Chemical Physics*, **2016**, 18, 19557-66	3.6	83
93	Emergent Scalar and Vector Fields in Quantum Chemical Topology. *Challenges and Advances in Computational Chemistry and Physics*, **2016**, 131-150	0.7	7
92	Fermi and Coulomb correlation effects upon the interacting quantum atoms energy partition. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	17
91	An energy partition method based on localized molecular orbitals. *Computational and Theoretical Chemistry*, **2015**, 1053, 77-84	2	1
90	Revisiting the carbonyl n -⊠ 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
89	Dynamical correlation within the Interacting Quantum Atoms method through coupled cluster theory. *Computational and Theoretical Chemistry*, **2015**, 1053, 90-95	2	33
88	Efficient algorithms for Hirshfeld-I charges. *Journal of Chemical Physics*, **2015**, 143, 084115	3.9	7
87	One-electron images in real space: natural adaptive orbitals. *Journal of Computational Chemistry*, **2015**, 36, 833-43	3.5	25
86	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
85	On the interpretation of domain averaged Fermi hole analyses of correlated wavefunctions. *Physical Chemistry Chemical Physics*, **2014**, 16, 4586-97	3.6	23
84	Electron number distribution functions from molecular wavefunctions. Version 2. *Computer Physics Communications*, **2014**, 185, 2663-2682	4.2	18
83	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

82	Perspectives for quantum chemical topology in crystallography. *Physica Scripta*, **2013**, 87, 048106	2.6	5
81	Domain-averaged exchange-correlation energies as a physical underpinning for chemical graphs. *ChemPhysChem*, **2013**, 14, 1211-8	3.2	74
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	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
78	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
77	Beyond Standard Charge Density Topological Analyses **2011**, 303-358		6
76	Nature of Chemical Interactions from the Profiles of Electron Delocalization Indices. *Journal of Chemical Theory and Computation*, **2011**, 7, 1704-11	6.4	48
75	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
74	Electron number distribution functions with iterative Hirshfeld atoms. *Computational and Theoretical Chemistry*, **2011**, 975, 2-8	2	8
73	Generalized electron number distribution functions: real space versus orbital space descriptions. *Theoretical Chemistry Accounts*, **2011**, 128, 433-444	1.9	12
72	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
71	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
70	Steric repulsions, rotation barriers, and stereoelectronic effects: a real space perspective. *Journal of Computational Chemistry*, **2009**, 30, 98-109	3.5	74
69	Using pseudopotentials within the interacting quantum atoms approach. *Journal of Physical Chemistry A*, **2009**, 113, 7963-71	2.8	22
68	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
67	Theoretical Simulation of AlN Nanocrystals. *Journal of Physical Chemistry C*, **2008**, 112, 6667-6676	3.8	5
66	EDF: Computing electron number probability distribution functions in real space from molecular wave functions. *Computer Physics Communications*, **2008**, 178, 621-634	4.2	40
65	Electron□electron interactions between ELF basins. *Chemical Physics Letters*, **2008**, 454, 396-403	2.5	26

64	An electron number distribution view of chemical bonds in real space. *Physical Chemistry Chemical Physics*, **2007**, 9, 1087-92	3.6	57
63	Comparison of direct and flow integration based charge density population analyses. *Journal of Physical Chemistry A*, **2007**, 111, 12146-51	2.8	15
62	Spin resolved electron number distribution functions: how spins couple in real space. *Journal of Chemical Physics*, **2007**, 127, 144103	3.9	46
61	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
60	Bond paths as privileged exchange channels. *Chemistry - A European Journal*, **2007**, 13, 9362-71	4.8	260
59	Chemical fragments in real space: definitions, properties, and energetic decompositions. *Journal of Computational Chemistry*, **2007**, 28, 161-84	3.5	119
58	Spatial localization, correlation, and statistical dependence of electrons in atomic domains: The . *Chemical Physics Letters*, **2007**, 437, 287-292	2.5	19
57	Electron number probability distributions for correlated wave functions. *Journal of Chemical Physics* , **2007**, 126, 094102	3.9	66
56	Pauling resonant structures in real space through electron number probability distributions. *Journal of Physical Chemistry A*, **2007**, 111, 1084-90	2.8	40
55	A Molecular Energy Decomposition Scheme for Atoms in Molecules. *Journal of Chemical Theory and Computation*, **2006**, 2, 90-102	6.4	232
54	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
53	The nature of the hydrogen bond: a synthesis from the interacting quantum atoms picture. *Journal of Chemical Physics*, **2006**, 125, 184112	3.9	183
52	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
51	Revisiting the variational nature of the quantum theory of atoms in molecules. *Chemical Physics Letters*, **2006**, 417, 16-21	2.5	17
50	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
49	Global optimization of ionic Mg(n)F(2n) (n=1-30) clusters. *Journal of Chemical Physics*, **2005**, 123, 234305	3.9	14
48	Evolution of the properties of Al(n)N(n) clusters with size. *Journal of Physical Chemistry B*, **2005**, 109, 24352-60	3.4	39
47	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

46	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
45	Reduced-size representations of high-quality atomic densities. The hybrid Gaussian□exponential case. *Theoretical Chemistry Accounts*, **2004**, 112, 113	1.9	
44	GIBBS: isothermal-isobaric thermodynamics of solids from energy curves using a quasi-harmonic Debye model. *Computer Physics Communications*, **2004**, 158, 57-72	4.2	1309
43	Two-electron integrations in the quantum theory of atoms in molecules. *Journal of Chemical Physics* , **2004**, 120, 4581-92	3.9	143
42	Spinodal equation of state for rutile TiO2. *Physical Review B*, **2003**, 67,	3.3	6
41	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
40	First-principles study of the rocksalt□esium chloride relative phase stability in alkali halides. *Physical Review B*, **2002**, 66,	3.3	432
39	Atomistic Simulation of the Equation of State of SrF 2 Using Electron Gas Interionic Potentials. *High Pressure Research*, **2002**, 22, 227-230	1.6	3
38	Microscopic Study of the Rock Salt-Caesium Chloride Phase Stability in Alkali Halides. *High Pressure Research*, **2002**, 22, 443-446	1.6	1
37	Hirshfeld surfaces as approximations to interatomic surfaces. *Journal of Chemical Physics*, **2002**, 117, 1017-1023	3.9	31
36	Quantum-mechanical analysis of the equation of state of anatase TiO2. *Physical Review B*, **2001**, 64,	3.3	63
35	Atomistic simulation of SrF2 polymorphs. *Physical Review B*, **2001**, 63,	3.3	435
34	Structure and Bonding in Magnesium Difluoride Clusters: The MgF2 Molecule. *Journal of Physical Chemistry A*, **2001**, 105, 4126-4135	2.8	10
33	A Theoretical Study of the Cluster Vibrations in Cr2O2, Cr2O3, and Cr2O4. *Journal of Physical Chemistry A*, **2000**, 104, 990-994	2.8	27
32	Strategies for determining and using ab initio interionic potentials. *Radiation Effects and Defects in Solids*, **1999**, 151, 223-228	0.9	3
31	Quantum-Mechanical Study of Thermodynamic and Bonding Properties of MgF2. *Journal of Physical Chemistry A*, **1998**, 102, 1595-1601	2.8	374
30	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
29	Thermodynamical properties of solids from microscopic theory: applications to MgF2 and Al2O3. *Computational and Theoretical Chemistry*, **1996**, 368, 245-255		452

28	Atomistic simulation of the pressure-temperature-volume diagram in Al2O3. *Solid State Communications*, **1996**, 98, 41-44	1.6	7
27	Energetics of the RbF + CaF2 -lRbCaF3 solid state reaction: A first-principles study. *Radiation Effects and Defects in Solids*, **1995**, 134, 193-196	0.9	1
26	Inference of crystal properties from cluster magnitudes. *Journal of Chemical Physics*, **1995**, 103, 432-439	3.9	4
25	Modeling the O2--O2- interaction for atomistic simulations. *Physical Review B*, **1995**, 51, 11289-11295	3.3	7
24	Stability of B1 and B2 phases from electronic density topology considerations. *Radiation Effects and Defects in Solids*, **1995**, 134, 201-203	0.9	
23	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	
22	Derivation of electron-gas interatomic potentials from quantum-mechanical descriptions of ions in crystals. *Physical Review B*, **1995**, 51, 2703-2714	3.3	23
21	Theoretical study of the coordination of the Cr3+ ion in Al2O3. *Radiation Effects and Defects in Solids*, **1995**, 134, 123-126	0.9	1
20	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
19	Ab initio pair potentials from quantum-mechanical atoms-in-crystals calculations. *Journal of Physics Condensed Matter*, **1993**, 5, 4975-4988	1.8	11
18	Low- and high-pressure ab initio equations of state for the alkali chlorides. *Physical Review B*, **1993**, 48, 5891-5901	3.3	41
17	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
16	Exact versus truncated spectrally resolved exchange in ab initio calculations. *Journal of Chemical Physics*, **1992**, 97, 452-458	3.9	5
15	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		7
14	Generalized Huzinaga building-block equations for nonorthogonal electronic groups: Relation to the AdamsGilbert theory. *Journal of Chemical Physics*, **1992**, 97, 6504-6508	3.9	50
13	Overlap, effective-potential, and projection-operator bicentric integrals over complex Slater-type orbitals. *Physical Review A*, **1991**, 43, 3384-3391	2.6	13
12	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	0.9	
11	Theoretical d-d spectrum of Cr3+:Mg0. *Radiation Effects and Defects in Solids*, **1991**, 119-121, 437-438	0.9	

10	Local wave functions for multinegative ions in solids. *Radiation Effects and Defects in Solids*, **1991**, 119-121, 727-728	0.9	
9	Theoretical spin-orbit coupling constants for 3d ions in crystals. *Physical Review B*, **1988**, 37, 5278-5288	3.3	17
8	The coulombic lattice potential of ionic compounds: The cubic perovskites. *Journal of Chemical Education*, **1988**, 65, 6	2.4	5
7	Accurate calculation of spin-orbit coupling constants for 3d atoms and ions with effective core potentials and reduced basis sets. *Physical Review A*, **1987**, 36, 1978-1982	2.6	16
6	Reduction of orbital sets. *Computer Physics Communications*, **1987**, 43, 269-277	4.2	2
5	Basis sets generation: Relation between Adamowicz and the maximum overlap method. *International Journal of Quantum Chemistry*, **1987**, 31, 279-285	2.1	3
4	Core projection effects in near-ab-initio valence calculations: II. Ground state geometry of octahedral chromium (I, II, III, and IV) hexafluorides. *Journal of Solid State Chemistry*, **1987**, 66, 263-282	3.3	14
3	3d-4s and 3d-4p electronic transitions in M2+ : NaF AND M2+ : KMgF3 (V, Cr, and Mn). Results of a cluster-model calculation. *Journal De Chimie Physique Et De Physico-Chimie Biologique*, **1987**, 84, 855-861		3
2	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		7
1	The maximum overlap method: A general and efficient scheme for reducing basis sets. Application to the generation of approximate AO for the 3d transition metal atoms and ions. *Journal of Solid State Chemistry*, **1986**, 63, 391-400	3.3	16