

# Luis Lain

## List of Publications by Year in descending order

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citations

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122  
docs citations

122  
times ranked

622  
citing authors

#	ARTICLE	IF	CITATIONS
1	Multicenter bonding within the AIM theory. <i>Theoretical Chemistry Accounts</i> , 2001, 105, 292-298.	0.5	86
2	On the definition of bond orders at correlated level. <i>Chemical Physics Letters</i> , 2003, 374, 567-571.	1.2	52
3	On the density matrix of effectively unpaired electrons. <i>Chemical Physics Letters</i> , 2001, 346, 283-287.	1.2	51
4	Variational Optimization of the Second-Order Density Matrix Corresponding to a Seniority-Zero Configuration Interaction Wave Function. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4064-4076.	2.3	46
5	Bond Orders and Their Relationships with Cumulant and Unpaired Electron Densities. <i>Journal of Physical Chemistry A</i> , 2003, 107, 127-130.	1.1	45
6	Configuration interaction wave functions: A seniority number approach. <i>Journal of Chemical Physics</i> , 2014, 140, 234103.	1.2	39
7	Pair Population Analysis within AIM Theory. <i>Journal of Physical Chemistry A</i> , 2000, 104, 9130-9135.	1.1	37
8	Seniority number in spin-adapted spaces and compactness of configuration interaction wave functions. <i>Journal of Chemical Physics</i> , 2013, 139, 084103.	1.2	37
9	A hybrid configuration interaction treatment based on seniority number and excitation schemes. <i>Journal of Chemical Physics</i> , 2014, 141, 244118.	1.2	36
10	On the Physical Meaning of Bond Indices from the Population Analysis of Higher Order Densities. <i>Journal of Physical Chemistry A</i> , 1998, 102, 7176-7180.	1.1	35
11	Local spin: A treatment beyond single determinant wave functions. <i>Chemical Physics Letters</i> , 2009, 470, 136-139.	1.2	34
12	Energy decompositions according to physical space partitioning schemes. <i>Journal of Chemical Physics</i> , 2005, 122, 074102.	1.2	33
13	Atomic valence in molecular systems. <i>Chemical Physics Letters</i> , 2003, 375, 45-53.	1.2	32
14	Studies of Population Analysis at the Correlated Level: Determination of Three-Center Bond Indices. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4132-4137.	1.1	32
15	Determination of Local Spins by Means of a Spin-Free Treatment. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3560-3566.	2.3	32
16	On the definition of the spin-free cumulant of the second-order reduced density matrix. <i>Journal of Chemical Physics</i> , 2002, 117, 5497-5498.	1.2	31
17	On the Nature of C <sup>+</sup> -Li Bonding in Lithiated Hydrocarbons and Lithiocarbons. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1019-1025.	1.1	30
18	On the measure of electron correlation and entanglement in quantum chemistry based on the cumulant of the second-order reduced density matrix. <i>Journal of Chemical Physics</i> , 2010, 133, 144104.	1.2	28

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19	On the definition of the effectively unpaired electron density matrix: A similarity measure approach. <i>Chemical Physics Letters</i> , 2006, 429, 286-288.	1.2	27
20	A study of the partitioning of the first-order reduced density matrix according to the theory of atoms in molecules. <i>Journal of Chemical Physics</i> , 2005, 123, 144113.	1.2	26
21	Electron-density topology in molecular systems: Paired and unpaired densities. <i>Journal of Chemical Physics</i> , 2005, 123, 144116.	1.2	25
22	Direct variational determination of the two-electron reduced density matrix for doubly occupied-configuration-interaction wave functions: The influence of three-index $\langle i   N   i \rangle$ -representability conditions. <i>Journal of Chemical Physics</i> , 2018, 148, 024105.	1.2	25
23	Topological Population Analysis from Higher Order Densities II. The Correlated Case. <i>Journal of Mathematical Chemistry</i> , 2002, 32, 241-248.	0.7	24
24	Polynomial scaling approximations and dynamic correlation corrections to doubly occupied configuration interaction wave functions. <i>Journal of Chemical Physics</i> , 2015, 143, 104106.	1.2	24
25	On the nature of multicenter bonding in simple atomic clusters. <i>Computational and Theoretical Chemistry</i> , 2000, 505, 283-288.	1.5	23
26	Topological population analysis from higher order densities. I. Hartree-Fock level. <i>Journal of Mathematical Chemistry</i> , 2000, 28, 83-90.	0.7	23
27	Comment on "Characterizing unpaired electrons from one-particle density matrix" [M. Head-Gordon, <i>Chem. Phys. Lett.</i> 372 (2003) 508-511]. <i>Chemical Physics Letters</i> , 2003, 380, 486-487.	1.2	23
28	Determination of Three-Center Bond Indices from Population Analyses: A Fuzzy Atom Treatment. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6587-6591.	1.1	23
29	An orbital localization criterion based on the theory of "fuzzy" atoms. <i>Journal of Computational Chemistry</i> , 2006, 27, 596-608.	1.5	23
30	Matrix elements of the third-order spin-adapted reduced Hamiltonian. <i>Physical Review A</i> , 1988, 38, 2721-2728.	1.0	22
31	Treatments of non-nuclear attractors within the theory of atoms in molecules. <i>Chemical Physics Letters</i> , 2005, 407, 379-383.	1.2	21
32	Relationships between Cumulant and Spin-Density Matrices: Application to the Decomposition of Spin. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2344-2349.	1.1	21
33	Reactive and inelastic processes involving $I_2(D^+ + u)$ with the collision partners CH <sub>4</sub> , CH <sub>3</sub> Cl, CF <sub>3</sub> Cl, and CF <sub>4</sub> . <i>Journal of Chemical Physics</i> , 1983, 78, 3727-3731.	1.2	20
34	Laplacian Field of the Effectively Unpaired Electron Density: Determination of Many-Body Effects on Electron Distributions. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3166-3172.	1.1	19
35	Calculation of traces of p-order replacement operators over N-electron spin-adapted spaces. <i>Physical Review A</i> , 1993, 47, 923-928.	1.0	18
36	A decomposition of the number of effectively unpaired electrons and its physical meaning. <i>Chemical Physics Letters</i> , 2009, 476, 101-103.	1.2	17

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37	Performance of Shannon-entropy compacted N-electron wave functions for configuration interaction methods. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	16
38	A study of the relationships between unpaired electron density, spin-density and cumulant matrices. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 405-410.	0.5	15
39	Chemical bonding analysis in boron clusters by means of localized orbitals according to the electron localization function topology. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	15
40	Correlated holes and their relationships with reduced density matrices and cumulants. <i>Journal of Chemical Physics</i> , 2005, 122, 084117.	1.2	14
41	Covalent bond orders revisited: the open-shell case. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 5144.	1.3	14
42	Electronic Structure and Effectively Unpaired Electron Density Topology in <i>closo</i> -Boranes: Nonclassical Three-Center Two-Electron Bonding. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 979-987.	2.3	14
43	Variational reduced density matrix method in the doubly occupied configuration interaction space using three-particle <i>N</i> -representability conditions. <i>Journal of Chemical Physics</i> , 2018, 149, 194105.	1.2	14
44	Magnetic Properties of Mononuclear Co(II) Complexes with Carborane Ligands. <i>Inorganic Chemistry</i> , 2018, 57, 7763-7769.	1.9	14
45	Generalization to <i>n</i> -th order space of the independent-pair model, within the spin-adapted reduced-Hamiltonian theoretical framework. <i>Physical Review A</i> , 1988, 37, 2868-2871.	1.0	13
46	Topology of the Effectively Paired and Unpaired Electron Densities for Complex Bonding Patterns: The Three-Center Two-Electron Bonding Case. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2030-2043.	2.3	13
47	Descriptions of local spins in the three-dimensional physical space. <i>Chemical Physics Letters</i> , 2011, 504, 236-240.	1.2	13
48	Fukui and dual-descriptor matrices within the framework of spin-polarized density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 9594.	1.3	13
49	Atom and Bond Fukui Functions and Matrices: A Hirshfeld's Atoms-in-Molecule Approach. <i>ChemPhysChem</i> , 2016, 17, 2881-2889.	1.0	13
50	Variational reduced density matrix method in the doubly-occupied configuration interaction space using four-particle <i>N</i> -representability conditions: Application to the XXZ model of quantum magnetism. <i>Journal of Chemical Physics</i> , 2019, 151, 154104.	1.2	13
51	Third-order many-body perturbation theory for intermolecular interactions. I. Hartree-Fock level. , 1997, 64, 43-51.		12
52	Energy decompositions according to physical space partitioning schemes: Treatments of the density cumulant. <i>Journal of Chemical Physics</i> , 2007, 127, 104110.	1.2	12
53	Topology of the Electron Density in Open-Shell Systems. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1200-1206.	1.1	12
54	Direct computation of traces of <i>n</i> -order replacement operators over <i>N</i> -electron spin-adapted spaces. <i>Physical Review A</i> , 1995, 52, 2446-2448.	1.0	11

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55	Covalent bond indices and ionicities from similarity measures. <i>Chemical Physics Letters</i> , 2007, 442, 157-163.	1.2	11
56	Electronic structure studies of diradicals derived from Closo-Carboranes. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	11
57	An orbital localization criterion based on the topological analysis of the electron localization function. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1401-1408.	1.0	11
58	Magnetic Properties of Co(II) Complexes with Polyhedral Carborane Ligands. <i>Inorganic Chemistry</i> , 2019, 58, 2550-2557.	1.9	11
59	Unrestricted treatment for the direct variational determination of the two-electron reduced density matrix for doubly occupied-configuration-interaction wave functions. <i>Journal of Chemical Physics</i> , 2019, 150, 164106.	1.2	11
60	Direct approximation to the reduced density matrices: Calculation of the isoelectronic sequence of beryllium up to argon. <i>Physical Review A</i> , 1986, 33, 1525-1531.	1.0	10
61	Representation of the spin operator in the spin-free second quantized approach. <i>Computational and Theoretical Chemistry</i> , 1998, 426, 25-28.	1.5	10
62	Nature of nonclassical bonds in Closo-Boranes: Nonlinear population analysis approach. <i>Journal of Computational Chemistry</i> , 1999, 20, 1085-1090.	1.5	10
63	Decomposition of the First-Order Reduced Density Matrix: An Isopycnic Localization Treatment. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9254-9260.	1.1	10
64	Orbital Localization Criterion as a Complementary Tool in the Bonding Analysis by Means of Electron Localization Function: Study of the Si <sub>n</sub> (BH) <sub>5-n</sub> <sup>2-</sup> (<i>n</i>). <i>Theoretical Chemistry Accounts</i> , 2010, 119, 1000-1006.	1.0	10
65	Toward (car)borane-based molecular magnets. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	10
66	Spin-adapted reduced-Hamiltonian theory: Application of the independent-pair model to the isoelectronic sequence of lithium. <i>Physical Review A</i> , 1987, 35, 3132-3135.	1.0	9
67	Multicenter bonding in open-shell systems. A nonlinear population analysis approach. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 710-715.	1.0	9
68	Determination of atomic valence indices from population analyses at correlated level. <i>Journal of Computational Chemistry</i> , 2003, 24, 1902-1909.	1.5	9
69	Treatment of non-nuclear attractors within the theory of atoms in molecules II: Energy decompositions. <i>Chemical Physics Letters</i> , 2006, 426, 426-430.	1.2	9
70	Grand-canonical-ensemble representability problem for the one-electron reduced density matrix. <i>Physical Review A</i> , 2007, 75, .	1.0	9
71	Description of functional groups by means of domain-restricted reduced density matrices. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 827-835.	0.5	9
72	Fukui and dual-descriptor matrices in the basis-set representation: A spin-free approach. <i>Chemical Physics Letters</i> , 2012, 533, 114-117.	1.2	9

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73	Spin contamination-free N-electron wave functions in the excitation-based configuration interaction treatment. <i>Journal of Chemical Physics</i> , 2016, 145, 014109.	1.2	8
74	Hybrid Treatments Based on Determinant Seniority Numbers and Spatial Excitation Levels in the Configuration Interaction Framework. <i>Advances in Quantum Chemistry</i> , 2018, , 315-332.	0.4	8
75	Analysis of Local and Global Aromaticity in Si <sub>3</sub> C <sub>5</sub> and Si <sub>4</sub> C <sub>8</sub> Clusters. <i>Aromatic Species Containing Planar Tetracoordinate Carbon. Chemistry</i> , 2021, 3, 1101-1112.	0.9	7
76	Competition between reactive and inelastic processes involving I <sub>2</sub> (D <sub>1</sub> <sup>h</sup> +u). <i>Chemical Physics Letters</i> , 1982, 91, 491-493.	1.2	6
77	Second-order spin-adapted reduced Hamiltonian in the coordinate representation. <i>Physical Review A</i> , 1989, 39, 4967-4971.	1.0	6
78	Variational determination of the two-particle reduced density matrix within the doubly occupied configuration interaction space: exploiting translational and reflection invariance. <i>Journal of Statistical Mechanics: Theory and Experiment</i> , 2021, 2021, 013110.	0.9	6
79	Ground and excited state similarity studies by means of Fukui and dual-descriptor matrices. <i>Chemical Physics Letters</i> , 2012, 549, 103-107.	1.2	5
80	A study of the compactness of wave functions based on Shannon entropy indices: a seniority number approach. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	5
81	Incorporating dynamic correlation into the variational determination method of the second-order reduced density matrix in the doubly occupied configuration interaction space. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26256.	1.0	5
82	Calculation of moments of spectral density distributions in finite-dimensional N-electron spin-adapted spaces. <i>Journal of Physics A</i> , 1995, 28, 271-279.	1.6	4
83	Determination of Energies and Electronic Densities of Functional Groups According to Partitionings in the Physical Space. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10023-10028.	1.1	4
84	An orbital localization criterion based on the topological analysis of the electron localization function at correlated level. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25588.	1.0	4
85	Variational determination of the two-electron reduced density matrix within the doubly occupied configuration interaction scheme: An extension to the study of open-shell systems. <i>Journal of Chemical Physics</i> , 2020, 153, 084101.	1.2	4
86	Variational determination of ground and excited-state two-electron reduced density matrices in the doubly occupied configuration space: A dispersion operator approach. <i>Journal of Chemical Physics</i> , 2021, 154, 224104.	1.2	4
87	A new partitioning of the total energy and its application to an analysis of a non-variational approach to many-electron theory. <i>Chemical Physics Letters</i> , 1988, 147, 219-222.	1.2	3
88	A formal construction of the N-electron Hamiltonian matrix and its blocks factorization. <i>Societa Italiana Di Fisica Nuovo Cimento B-General Physics, Relativity Astronomy and Mathematical Physics and Methods</i> , 1991, 106, 1079-1084.	0.2	3
89	Calculation of the dimension of full configuration interaction spaces: application to the determination of spectroscopic terms. <i>Computational and Theoretical Chemistry</i> , 1993, 287, 63-66.	1.5	3
90	Symmetry-adapted formulation of the combined G-particle-hole hypervirial equation and Hermitian operator method. <i>Journal of Mathematical Chemistry</i> , 2014, 52, 1794-1806.	0.7	3

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91	Determination of heisenberg exchange coupling constants in clusters with magnetic sites: A local spin approach. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 952-958.	1.0	3
92	Determination of exchange coupling constants in linear polyradicals by means of local spins. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	3
93	A note on dirac's time-dependent perturbation theory. <i>Chemical Physics Letters</i> , 1981, 84, 583-586.	1.2	2
94	A general iterative time-independent perturbation theory. <i>Canadian Journal of Physics</i> , 1985, 63, 1157-1161.	0.4	2
95	A simple derivation of the series in perturbation theory. <i>European Journal of Physics</i> , 1987, 8, 178-181.	0.3	2
96	Calculation of traces of Hamiltonian powers in finite-dimensional N-electron spin-adapted spaces: application to the determination of moments of spectral density distributions. <i>Journal of Physics A</i> , 1995, 28, 3363-3370.	1.6	2
97	Domain-averaged Fermi hole and domain-restricted reduced density matrices: A critical comparison. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 256-262.	1.0	2
98	Electronic densities in systems with fractionally charged nuclei: a symmetry breaking study. <i>Journal of Mathematical Chemistry</i> , 2015, 53, 236-249.	0.7	2
99	Molecular magnetism in closo-azadodecaborane supericosahedrons. <i>Molecular Physics</i> , 2015, , 1-7.	0.8	2
100	Magnetic properties of closo-carborane-based Co(II) single-ion complexes with O, S, Se, and Te bridging atoms. <i>Polyhedron</i> , 2020, 176, 114257.	1.0	2
101	Molecular Energy Decompositions in the Hilbert-Space of Atomic Orbitals at Correlated Level. <i>Progress in Theoretical Chemistry and Physics</i> , 2008, , 203-214.	0.2	2
102	Precipitation chromatography fractionation: The effect of the ratio support weight/sample size. <i>European Polymer Journal</i> , 1978, 14, 991-994.	2.6	1
103	Radial probability density and normalization in hydrogenic atoms. <i>Journal of Chemical Education</i> , 1981, 58, 617.	1.1	1
104	Does quantum mechanics apply to one or many particles?. <i>Journal of Chemical Education</i> , 1983, 60, 377.	1.1	1
105	A practical iterative method in time-independent perturbation theory. <i>Societa Italiana Di Fisica Nuovo Cimento B-General Physics, Relativity Astronomy and Mathematical Physics and Methods</i> , 1985, 86, 83-89.	0.2	1
106	Traces of pth-order reduced density matrices: symmetric group approach. <i>Journal of Physics A</i> , 1998, 31, 5811-5817.	1.6	1
107	Exploiting the nearsightedness principle within the framework of the anti-Hermitian contracted Schrödinger equation. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	1
108	Variational determination of the two-electron reduced density matrix within the doubly occupied configuration interaction framework: Treatments of triplet N-electron systems. <i>Journal of Chemical Physics</i> , 0, , .	1.2	1

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109	A theory of IR and other multiple photon dissociations. <i>Journal of Photochemistry and Photobiology</i> , 1981, 17, 178.	0.6	0
110	Have quantum mechanical isolated systems a physical meaning? An essential approximation in basic quantum physics. <i>European Journal of Physics</i> , 1983, 4, 107-109.	0.3	0
111	The role of collisions in the fate of excited states. <i>Journal of Chemical Education</i> , 1984, 61, 636.	1.1	0
112	Contraction algorithms for third-order reduced density matrices: Symmetric group approach. <i>Journal of Mathematical Chemistry</i> , 1993, 13, 177-189.	0.7	0
113	A criterion for determining a finite basis set for calculating potential energy curves and surfaces. <i>Computational and Theoretical Chemistry</i> , 1993, 287, 47-53.	1.5	0
114	Analysis of several methods in the direct approximation of reduced density matrices. <i>Societa Italiana Di Fisica Nuovo Cimento B-General Physics, Relativity Astronomy and Mathematical Physics and Methods</i> , 1993, 108, 491-498.	0.2	0
115	Matrix elements of Sz-adapted and theLz-adapted reduced Hamiltonians. <i>Computational and Theoretical Chemistry</i> , 1995, 330, 41-47.	1.5	0
116	Determination of spectroscopic terms in the LS-coupling scheme: a full configuration interaction space approach. <i>Computational and Theoretical Chemistry</i> , 1995, 330, 197-200.	1.5	0
117	Traces of Hamiltonian powers in N-electron model spaces. <i>Computational and Theoretical Chemistry</i> , 1998, 426, 29-33.	1.5	0
118	A general determination of the energy averaged over spin-adapted atomic states. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 1998, 31, 4259-4265.	0.6	0
119	Analysis of molecular and (di)atomic dual-descriptor functions and matrices. <i>Journal of Molecular Modeling</i> , 2017, 23, 185.	0.8	0
120	Electronic and structural relations between solid CaB6 and the molecular dianion B6H6(2-): A computational study. <i>Solid State Sciences</i> , 2020, 102, 106169.	1.5	0
121	Symmetry-adapted formulation of the hybrid treatment resulting from the G-particle-hole Hypervirial equation and equations of motion methods: a procedure for modeling solids. <i>Journal of Mathematical Chemistry</i> , 2021, 59, 488-504.	0.7	0
122	Comment on "Study of counterintuitive transport properties in the Aubry-Andr�-Harper model via entanglement entropy and persistent current". <i>Physical Review B</i> , 2020, 101, .	1.1	0