Luis Lain

List of Publications by Year
in descending order

122 papers	1,658 citations	279701 23 h-index	395590 33 g-index
122 all docs	122 docs citations	122 times ranked	622 citing authors

#	Article	IF	Citations
1	Exploiting the nearsightedness principle within the framework of the antiâ€Hermitian contracted SchrÃ¶dinger equation. International Journal of Quantum Chemistry, 2022, 122, .	1.0	1
2	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. Journal of Mathematical Chemistry, 2021, 59, 488-504.	0.7	0
3	Variational determination of ground and excited-state two-electron reduced density matrices in the doubly occupied configuration space: A dispersion operator approach. Journal of Chemical Physics, 2021, 154, 224104.	1.2	4
4	Analysis of Local and Global Aromaticity in Si3C5 and Si4C8 Clusters. Aromatic Species Containing Planar Tetracoordinate Carbon. Chemistry, 2021, 3, 1101-1112.	0.9	7
5	Variational determination of the two-particle reduced density matrix within the doubly occupied configuration interaction space: exploiting translational and reflection invariance. Journal of Statistical Mechanics: Theory and Experiment, 2021, 2021, 013110.	0.9	6
6	Magnetic properties of closo-carborane-based Co(II) single-ion complexes with O, S, Se, and Te bridging atoms. Polyhedron, 2020, 176, 114257.	1.0	2
7	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. Journal of Chemical Physics, 2020, 153, 084101.	1.2	4
8	Electronic and structural relations between solid CaB6 and the molecular dianion B6H6(2-): A computational study. Solid State Sciences, 2020, 102, 106169.	1.5	0
9	Incorporating dynamic correlation into the variational determination method of the secondâ€order reduced density matrix in the doubly occupied configuration interaction space. International Journal of Quantum Chemistry, 2020, 120, e26256.	1.0	5
10	Comment on â€œStudy of counterintuitive transport properties in the Aubry-AndrÃ©-Harper model via entanglement entropy and persistent currentâ€• Physical Review B, 2020, 101, .	1.1	0
11	Magnetic Properties of Co(II) Complexes with Polyhedral Carborane Ligands. Inorganic Chemistry, 2019, 58, 2550-2557.	1.9	11
12	Unrestricted treatment for the direct variational determination of the two-electron reduced density matrix for doubly occupied-configuration-interaction wave functions. Journal of Chemical Physics, 2019, 150, 164106.	1.2	11
13	Variational reduced density matrix method in the doubly-occupied configuration interaction space using four-particle N-representability conditions: Application to the XXZ model of quantum magnetism. Journal of Chemical Physics, 2019, 151, 154104.	1.2	13
14	An orbital localization criterion based on the topological analysis of the electron localization function at correlated level. International Journal of Quantum Chemistry, 2018, 118, e25588.	1.0	4
15	Direct variational determination of the two-electron reduced density matrix for doubly occupied-configuration-interaction wave functions: The influence of three-index N-representability conditions. Journal of Chemical Physics, 2018, 148, 024105.	1.2	25
16	Variational reduced density matrix method in the doubly occupied configuration interaction space using three-particle N-representability conditions. Journal of Chemical Physics, 2018, 149, 194105.	1.2	14
17	Hybrid Treatments Based on Determinant Seniority Numbers and Spatial Excitation Levels in the Configuration Interaction Framework. Advances in Quantum Chemistry, 2018, , 315-332.	0.4	8
18	Magnetic Properties of Mononuclear Co(II) Complexes with Carborane Ligands. Inorganic Chemistry, 2018, 57, 7763-7769.	1.9	14

#	Article	IF	Citations
19	Analysis of molecular and (di)atomic dual-descriptor functions and matrices. Journal of Molecular Modeling, 2017, 23, 185.	0.8	0
20	Determination of exchange coupling constants in linear polyradicals by means of local spins. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	3
21	Spin contamination-free N-electron wave functions in the excitation-based configuration interaction treatment. Journal of Chemical Physics, 2016, 145, 014109.	1.2	8
22	Performance of Shannon-entropy compacted N-electron wave functions for configuration interaction methods. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	16
23	Atom and Bond Fukui Functions and Matrices: A Hirshfeldâ€ Atomsâ€inâ€Molecule Approach. ChemPhysChem, 2016, 17, 2881-2889.	1.0	13
24	Chemical bonding analysis in boron clusters by means of localized orbitals according to the electron localization function topology. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	15
25	Electronic densities in systems with fractionally charged nuclei: a symmetry breaking study. Journal of Mathematical Chemistry, 2015, 53, 236-249.	0.7	2
26	A study of the compactness of wave functions based on Shannon entropy indices: a seniority number approach. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	5
27	Variational Optimization of the Second-Order Density Matrix Corresponding to a Seniority-Zero Configuration Interaction Wave Function. Journal of Chemical Theory and Computation, 2015, 11, 4064-4076.	2.3	46
28	Toward (car)borane-based molecular magnets. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	10
29	Polynomial scaling approximations and dynamic correlation corrections to doubly occupied configuration interaction wave functions. Journal of Chemical Physics, 2015, 143, 104106.	1.2	24
30	Molecular magnetism incloso-azadodecaborane supericosahedrons. Molecular Physics, 2015, , 1-7.	0.8	2
31	A hybrid configuration interaction treatment based on seniority number and excitation schemes. Journal of Chemical Physics, 2014, 141, 244118.	1.2	36
32	Configuration interaction wave functions: A seniority number approach. Journal of Chemical Physics, 2014, 140, 234103.	1.2	39
33	Symmetry-adapted formulation of the combined G-particle-hole hypervirial equation and Hermitian operator method. Journal of Mathematical Chemistry, 2014, 52, 1794-1806.	0.7	3
34	Determination of heisenberg exchange coupling constants in clusters with magnetic sites: A local spin approach. International Journal of Quantum Chemistry, 2014, 114, 952-958.	1.0	3
35	Fukui and dual-descriptor matrices within the framework of spin-polarized density functional theory. Physical Chemistry Chemical Physics, 2013, 15, 9594.	1.3	13
36	Seniority number in spin-adapted spaces and compactness of configuration interaction wave functions. Journal of Chemical Physics, 2013, 139, 084103.	1.2	37

#	Article	IF	Citations
37	Orbital Localization Criterion as a Complementary Tool in the Bonding Analysis by Means of Electron Localization Function: Study of the Si_n(BH)_{5-n}²⁻ (n) Tj ETQq1 1 0.784314 rgBT /O		14
38	Electronic structure studies of diradicals derived from Closo-Carboranes. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	11
39	An orbital localization criterion based on the topological analysis of the electron localization function. International Journal of Quantum Chemistry, 2013, 113, 1401-1408.	1.0	11
40	Ground and excited state similarity studies by means of Fukui and dual-descriptor matrices. Chemical Physics Letters, 2012, 549, 103-107.	1.2	5
41	Fukui and dual-descriptor matrices in the basis-set representation: A spin-free approach. Chemical Physics Letters, 2012, 533, 114-117.	1.2	9
42	Electronic Structure and Effectively Unpaired Electron Density Topology in closo-Boranes: Nonclassical Three-Center Two-Electron Bonding. Journal of Chemical Theory and Computation, 2011, 7, 979-987.	2.3	14
43	Determination of Local Spins by Means of a Spin-Free Treatment. Journal of Chemical Theory and Computation, 2011, 7, 3560-3566.	2.3	32
44	A study of the relationships between unpaired electron density, spin-density and cumulant matrices. Theoretical Chemistry Accounts, 2011, 128, 405-410.	0.5	15
45	Domainâ€averaged Fermi hole and domainâ€restricted reduced density matrices: A critical comparison. International Journal of Quantum Chemistry, 2011, 111, 256-262.	1.0	2
46	Descriptions of local spins in the three-dimensional physical space. Chemical Physics Letters, 2011, 504, 236-240.	1.2	13
47	On the measure of electron correlation and entanglement in quantum chemistry based on the cumulant of the second-order reduced density matrix. Journal of Chemical Physics, 2010, 133, 144104.	1.2	28
48	Topology of the Electron Density in Open-Shell Systems. Journal of Physical Chemistry A, 2010, 114, 1200-1206.	1.1	12
49	Relationships between Cumulant and Spin-Density Matrices: Application to the Decomposition of Spin. Journal of Physical Chemistry A, 2010, 114, 2344-2349.	1.1	21
50	Local spin: A treatment beyond single determinant wave functions. Chemical Physics Letters, 2009, 470, 136-139.	1.2	34
51	A decomposition of the number of effectively unpaired electrons and its physical meaning. Chemical Physics Letters, 2009, 476, 101-103.	1.2	17
52	Topology of the Effectively Paired and Unpaired Electron Densities for Complex Bonding Patterns: The Three-Center Two-Electron Bonding Case. Journal of Chemical Theory and Computation, 2009, 5, 2030-2043.	2.3	13
53	Determination of Energies and Electronic Densities of Functional Groups According to Partitionings in the Physical Space. Journal of Physical Chemistry A, 2008, 112, 10023-10028.	1.1	4
54	Covalent bond orders revisited: the open-shell case. Physical Chemistry Chemical Physics, 2008, 10, 5144.	1.3	14

#	Article	IF	Citations
55	Molecular Energy Decompositions in the Hilbert-Space of Atomic Orbitals at Correlated Level. Progress in Theoretical Chemistry and Physics, 2008, , 203-214.	0.2	2
56	Energy decompositions according to physical space partitioning schemes: Treatments of the density cumulant. Journal of Chemical Physics, 2007, 127, 104110.	1.2	12
57	Grand-canonical-ensemble representability problem for the one-electron reduced density matrix. Physical Review A, 2007, 75, .	1.0	9
58	Laplacian Field of the Effectively Unpaired Electron Density:â€‰ Determination of Many-Body Effects on Electron Distributions. Journal of Physical Chemistry A, 2007, 111, 3166-3172.	1.1	19
59	Covalent bond indices and ionicities from similarity measures. Chemical Physics Letters, 2007, 442, 157-163.	1.2	11
60	Description of functional groups by means of domain-restricted reduced density matrices. Theoretical Chemistry Accounts, 2007, 118, 827-835.	0.5	9
61	Decomposition of the First-Order Reduced Density Matrix:â€‰ An Isopycnic Localization Treatment. Journal of Physical Chemistry A, 2006, 110, 9254-9260.	1.1	10
62	Treatment of non-nuclear attractors within the theory of atoms in molecules II: Energy decompositions. Chemical Physics Letters, 2006, 426, 426-430.	1.2	9
63	On the definition of the effectively unpaired electron density matrix: A similarity measure approach. Chemical Physics Letters, 2006, 429, 286-288.	1.2	27
64	An orbital localization criterion based on the theory of â€œfuzzyâ€•atoms. Journal of Computational Chemistry, 2006, 27, 596-608.	1.5	23
65	Treatments of non-nuclear attractors within the theory of atoms in molecules. Chemical Physics Letters, 2005, 407, 379-383.	1.2	21
66	A study of the partitioning of the first-order reduced density matrix according to the theory of atoms in molecules. Journal of Chemical Physics, 2005, 123, 144113.	1.2	26
67	Energy decompositions according to physical space partitioning schemes. Journal of Chemical Physics, 2005, 122, 074102.	1.2	33
68	Correlated holes and their relationships with reduced density matrices and cumulants. Journal of Chemical Physics, 2005, 122, 084117.	1.2	14
69	Determination of Three-Center Bond Indices from Population Analyses:â€‰ A Fuzzy Atom Treatment. Journal of Physical Chemistry A, 2005, 109, 6587-6591.	1.1	23
70	Electron-density topology in molecular systems: Paired and unpaired densities. Journal of Chemical Physics, 2005, 123, 144116.	1.2	25
71	Studies of Population Analysis at the Correlated Level:Â Determination of Three-Center Bond Indices. Journal of Physical Chemistry A, 2004, 108, 4132-4137.	1.1	32
72	Determination of atomic valence indices from population analyses at correlated level. Journal of Computational Chemistry, 2003, 24, 1902-1909.	1.5	9

#	Article	IF	Citations
73	Comment on â€˜Characterizing unpaired electrons from one-particle density matrixâ€™ [M. Head-Gordon, Chem. Phys. Lett. 372 (2003) 508â€“511]. Chemical Physics Letters, 2003, 380, 486-487.	1.2	23
74	On the definition of bond orders at correlated level. Chemical Physics Letters, 2003, 374, 567-571.	1.2	52
75	Atomic valence in molecular systems. Chemical Physics Letters, 2003, 375, 45-53.	1.2	32
76	Bond Orders and Their Relationships with Cumulant and Unpaired Electron Densities. Journal of Physical Chemistry A, 2003, 107, 127-130.	1.1	45
77	On the Nature of Cî—¸Li Bonding in Lithiated Hydrocarbons and Lithiocarbons. Journal of Physical Chemistry A, 2002, 106, 1019-1025.	1.1	30
78	On the definition of the spin-free cumulant of the second-order reduced density matrix. Journal of Chemical Physics, 2002, 117, 5497-5498.	1.2	31
79	Topological Population Analysis from Higher Order Densities II. The Correlated Case. Journal of Mathematical Chemistry, 2002, 32, 241-248.	0.7	24
80	Multicenter bonding within the AIM theory. Theoretical Chemistry Accounts, 2001, 105, 292-298.	0.5	86
81	On the density matrix of effectively unpaired electrons. Chemical Physics Letters, 2001, 346, 283-287.	1.2	51
82	Multicenter bonding in open-shell systems. A nonlinear population analysis approach. International Journal of Quantum Chemistry, 2000, 77, 710-715.	1.0	9
83	On the nature of multicenter bonding in simple atomic clusters. Computational and Theoretical Chemistry, 2000, 505, 283-288.	1.5	23
84	Topological population analysis from higher order densities. I. Hartreeâ€“Fock level. Journal of Mathematical Chemistry, 2000, 28, 83-90.	0.7	23
85	Pair Population Analysis within AIM Theory. Journal of Physical Chemistry A, 2000, 104, 9130-9135.	1.1	37
86	Nature of nonclassical bonds in Closo-Boranes: Nonlinear population analysis approach. Journal of Computational Chemistry, 1999, 20, 1085-1090.	1.5	10
87	Representation of the spin operator in the spin-free second quantized approach. Computational and Theoretical Chemistry, 1998, 426, 25-28.	1.5	10
88	Traces of Hamiltonian powers in N-electron model spaces. Computational and Theoretical Chemistry, 1998, 426, 29-33.	1.5	0
89	On the Physical Meaning of Bond Indices from the Population Analysis of Higher Order Densities. Journal of Physical Chemistry A, 1998, 102, 7176-7180.	1.1	35
90	Traces ofpth-order reduced density matrices: symmetric group approach. Journal of Physics A, 1998, 31, 5811-5817.	1.6	1

#	Article	IF	Citations
91	A general determination of the energy averaged over spin-adapted atomic states. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 4259-4265.	0.6	0
92	Third-order many-body perturbation theory for intermolecular interactions. I. Hartree-Fock level. , 1997, 64, 43-51.		12
93	Matrix elements of Sz-adapted and theLz-adapted reduced Hamiltonians. Computational and Theoretical Chemistry, 1995, 330, 41-47.	1.5	0
94	Determination of spectroscopic terms in the LS-coupling scheme: a full configuration interaction space approach. Computational and Theoretical Chemistry, 1995, 330, 197-200.	1.5	0
95	Direct computation of traces ofp-order replacement operators overN-electron spin-adapted spaces. Physical Review A, 1995, 52, 2446-2448.	1.0	11
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. Journal of Physics A, 1995, 28, 3363-3370.	1.6	2
97	Calculation of moments of spectral density distributions in finite-dimensional N-electron spin-adapted spaces. Journal of Physics A, 1995, 28, 271-279.	1.6	4
98	Contraction algorithms for third-order reduced density matrices: Symmetric group approach. Journal of Mathematical Chemistry, 1993, 13, 177-189.	0.7	0
99	A criterion for determining a finite basis set for calculating potential energy curves and surfaces. Computational and Theoretical Chemistry, 1993, 287, 47-53.	1.5	0
100	Calculation of the dimension of full configuration interaction spaces: application to the determination of spectroscopic terms. Computational and Theoretical Chemistry, 1993, 287, 63-66.	1.5	3
101	Analysis of several methods in the direct approximation of reduced density matrices. Societa Italiana Di Fisica Nuovo Cimento B-General Physics, Relativity Astronomy and Mathematical Physics and Methods, 1993, 108, 491-498.	0.2	0
102	Calculation of traces ofp-order replacement operators overN-electron spin-adapted spaces. Physical Review A, 1993, 47, 923-928.	1.0	18
103	A formal construction of theN-electron Hamiltonian matrix and its blocks factorization. Societa Italiana Di Fisica Nuovo Cimento B-General Physics, Relativity Astronomy and Mathematical Physics and Methods, 1991, 106, 1079-1084.	0.2	3
104	Second-order spin-adapted reduced Hamiltonian in the coordinate representation. Physical Review A, 1989, 39, 4967-4971.	1.0	6
105	A new partitioning of the total energy and its application to an analysis of a non-variational approach to many-electron theory. Chemical Physics Letters, 1988, 147, 219-222.	1.2	3
106	Matrix elements of the third-order spin-adapted reduced Hamiltonian. Physical Review A, 1988, 38, 2721-2728.	1.0	22
107	Generalization to apth-order space of the independent-pair model, within the spin-adapted reduced-Hamiltonian theoretical framework. Physical Review A, 1988, 37, 2868-2871.	1.0	13
108	A simple derivation of the series in perturbation theory. European Journal of Physics, 1987, 8, 178-181.	0.3	2

#	Article	IF	Citations
109	Spin-adapted reduced-Hamiltonian theory: Application of the independent-pair model to the isoelectronic sequence of lithium. Physical Review A, 1987, 35, 3132-3135.	1.0	9
110	Direct approximation to the reduced density matrices: Calculation of the isoelectronic sequence of beryllium up to argon. Physical Review A, 1986, 33, 1525-1531.	1.0	10
111	A practical iterative method in time-independent perturbation theory. Societa Italiana Di Fisica Nuovo Cimento B-General Physics, Relativity Astronomy and Mathematical Physics and Methods, 1985, 86, 83-89.	0.2	1
112	A general iterative time-independent perturbation theory. Canadian Journal of Physics, 1985, 63, 1157-1161.	0.4	2
113	The role of collisions in the fate of excited states. Journal of Chemical Education, 1984, 61, 636.	1.1	0
114	Does quantum mechanics apply to one or many particles?. Journal of Chemical Education, 1983, 60, 377.	1.1	1
115	Have quantum mechanical isolated systems a physical meaning? An essential approximation in basic quantum physics. European Journal of Physics, 1983, 4, 107-109.	0.3	0
116	Reactive and inelastic processes involving I2(Dâ€‰1Î£+u) with the collision partners CH4, CH3Cl, CF3Cl, and CF4. Journal of Chemical Physics, 1983, 78, 3727-3731.	1.2	20
117	Competition between reactive and inelastic processes involving I2(D1Î£+u). Chemical Physics Letters, 1982, 91, 491-493.	1.2	6
118	Radial probability density and normalization in hydrogenic atoms. Journal of Chemical Education, 1981, 58, 617.	1.1	1
119	A note on dirac's time-dependent perturbation theory. Chemical Physics Letters, 1981, 84, 583-586.	1.2	2
120	A theory of IR and other multiple photon dissociations. Journal of Photochemistry and Photobiology, 1981, 17, 178.	0.6	0
121	Precipitation chromatography fractionation: The effect of the ratio support weight/sample size. European Polymer Journal, 1978, 14, 991-994.	2.6	1
122	Variational determination of the two-electron reduced density matrix within the doubly occupied configuration interaction framework: Treatments of triplet N-electron systems. Journal of Chemical Physics, 0, , .	1.2	1