Stefano Evangelisti

List of Publications by Year
in descending order

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113	2,516	218677	233421
papers	citations	26 h-index	45 g-index

114	114	114	1473
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Convergence of an improved CIPSI algorithm. Chemical Physics, 1983, 75, 91-102.	1.9	375
2	A vector and parallel full configuration interaction algorithm. Journal of Chemical Physics, 1993, 98, 3141-3150.	3.0	108
3	Direct generation of local orbitals for multireference treatment and subsequent uses for the calculation of the correlation energy. Journal of Chemical Physics, 2002, 116, 10060-10068.	3.0	107
4	3,5-Bis(ethynyl)pyridine and 2,6-Bis(ethynyl)pyridine Spanning Two Fe(Cp*)(dppe) Units: Role of the Nitrogen Atom on the Electronic and Magnetic Couplings. Inorganic Chemistry, 2011, 50, 12601-12622.	4.0	69
5	A theoretical study of the N 8 cubane to N 8 pentalene isomerization reaction. Theoretical Chemistry Accounts, 1997, 97, 136-142.	1.4	68
6	Dissociation reaction of N8 azapentalene to 4N2: A theoretical study. International Journal of Quantum Chemistry, 2000, 77, 311-315.	2.0	68
7	A theoretical study of the nitrogen clusters formed from the ions N3â^', N5+, and N5â^'. Journal of Chemical Physics, 2001, 114, 10733-10737.	3.0	67
8	Full configuration interaction calculations on Be2. Chemical Physics, 1994, 185, 47-56.	1.9	63
9	A novel perturbation-based complete active spaceâ€“self-consistent-field algorithm: Application to the direct calculation of localized orbitals. Journal of Chemical Physics, 2002, 117, 10525-10533.	3.0	61
10	A full-configuration benchmark for the N2 molecule. Chemical Physics Letters, 1999, 310, 530-536.	2.6	54
11	On the dissociation of N6 into 3 N2 molecules. Chemical Physics Letters, 2000, 320, 518-522.	2.6	47
12	Computation and analysis of the full configuration interaction wave function of some simple systems. International Journal of Quantum Chemistry, 1993, 48, 287-301.	2.0	45
13	Increasing Radical Character of Large [n]cyclacenes Unveiled by Wave Function Theory. Journal of Physical Chemistry A, 2017, 121, 3746-3756.	2.5	45
14	Beryllium Dimer: A Bond Based on Non-Dynamical Correlation. Journal of Physical Chemistry A, 2014, 118, 6664-6673.	2.5	44
15	A theoretical study of ten N8 isomers. Computational and Theoretical Chemistry, 1998, 428, 1-8.	1.5	41
16	Local Orbitals for the Truncation of Inactive Space:Â Application to Magnetic Systems. Journal of Physical Chemistry A, 2003, 107, 7581-7588.	2.5	40
17	The use of local orbitals in multireference calculations. Molecular Physics, 2003, 101, 1389-1398.	1.7	36
18	Full configuration interaction study of the metal-insulator transition in model systems: LiN linear chains (N=2,4,6,8). Journal of Chemical Physics, 2008, 128, 024701.	3.0	35

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19	A theoretical study of linear beryllium chains: Full configuration interaction. Journal of Chemical Physics, 2009, 130, 024301.	3.0	32
20	Exact entanglement entropy of the XYZ model and its sine-Gordon limit. Physics Letters, Section A: General, Atomic and Solid State Physics, 2010, 374, 2101-2105.	2.1	32
21	Nanostructure Selectivity for Molecular Adsorption and Separation: the Case of Graphyne Layers. Journal of Physical Chemistry C, 2018, 122, 16195-16208.	3.1	32
22	Direct-list algorithm for configuration interaction calculations. Journal of Computational Chemistry, 1997, 18, 1329-1343.	3.3	31
23	Full configuration interaction calculation of Be3. Journal of Chemical Physics, 2004, 120, 8405-8411.	3.0	31
24	A one billion determinant full CI benchmark on the Cray T3D. Chemical Physics Letters, 1996, 252, 437-446.	2.6	29
25	A parallel Full-CI algorithm. Computer Physics Communications, 2000, 128, 496-515.	7.5	29
26	A full CI algorithm on the CRAY T3D. Application to the NH3 molecule. Chemical Physics Letters, 1995, 233, 353-358.	2.6	27
27	The metal-insulator transition in dimerized HÃ¼ckel chains. Journal of Chemical Physics, 2008, 129, 134104.	3.0	26
28	Is HeHâ^' a stable system?. Chemical Physics, 1997, 215, 217-225.	1.9	24
29	Correlated description of multiple bonds using localized active orbitals. Chemical Physics Letters, 2001, 349, 555-561.	2.6	24
30	Can the second order multireference perturbation theory be considered a reliable tool to study mixed-valence compounds?. Journal of Chemical Physics, 2008, 128, 174102.	3.0	24
31	Abâ€initio multireference study of an organic mixedâ€valence Spiro molecular system. Journal of Computational Chemistry, 2009, 30, 83-92.	3.3	24
32	Kohnâ€™s localization in the insulating state: One-dimensional lattices, crystalline versus disordered. Journal of Chemical Physics, 2010, 133, 064703.	3.0	23
33	Ab Initio Study of Nitrogenâ^'Oxygen Clusters:Â N2O3, N4O6, and N8O12. Journal of Physical Chemistry A, 1998, 102, 4925-4929.	2.5	22
34	Multiple complete active space self-consistent field solutions. Molecular Physics, 2003, 101, 1937-1944.	1.7	22
35	Fullâ€configurationâ€interaction study of the metalâ€insulator transition in a model system: H_n linear chains n=4, 6,â€¦, 16. International Journal of Quantum Chemistry, 2011, 111, 3416-3423.	2.0	22
36	Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. Journal of Computational Chemistry, 2014, 35, 611-621.	3.3	22

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37	Ab initio potentials for weakly interacting systems: Homonuclear rare gas dimers. International Journal of Quantum Chemistry, 2003, 95, 303-312.	2.0	20
38	Signatures of Wigner localization in one-dimensional systems. Journal of Chemical Physics, 2018, 148, 124103.	3.0	20
39	Electron localizability and polarizability in tight-binding graphene nanostructures. Theoretical Chemistry Accounts, 2010, 126, 257-263.	1.4	19
40	Behavior of the Positionâ€“Spread Tensor in Diatomic Systems. Journal of Chemical Theory and Computation, 2013, 9, 5286-5295.	5.3	19
41	Full configuration interaction algorithm on a massively parallel architecture: Direct-list implementation. Journal of Computational Chemistry, 1998, 19, 658-672.	3.3	18
42	End states and singletâ€“triplet degeneracy in linear atomic chains. Chemical Physics Letters, 2008, 465, 102-105.	2.6	18
43	Asymptotic analysis of the localization spread and polarizability of 1â€Ð noninteracting electrons. International Journal of Quantum Chemistry, 2012, 112, 653-664.	2.0	18
44	A simple position operator for periodic systems. Physical Review B, 2019, 99, .	3.2	18
45	Localized molecular orbitals for excited states nâ†'Ï€* (CO) excitation. Chemical Physics Letters, 2003, 372, 22-27.	2.6	17
46	Ionic nitrogen clusters. Computational and Theoretical Chemistry, 2003, 621, 43-50.	1.5	16
47	Computing the Position-Spread tensor in the CAS-SCF formalism. Chemical Physics Letters, 2014, 591, 58-63.	2.6	16
48	The total position-spread tensor: Spin partition. Journal of Chemical Physics, 2015, 142, 094113.	3.0	16
49	Full configuration interaction study of the ground state of closed-shell cyclicPPP polyenes. International Journal of Quantum Chemistry, 1994, 51, 13-25.	2.0	15
50	Benchmark full-CI calculation on C2H2: comparison with (SC)2-CI and other truncated-CI approaches. Chemical Physics Letters, 1998, 288, 348-355.	2.6	15
51	The Effect of the Basis-Set Superposition Error on the Calculation of Dispersion Interactions:â€‰ A Test Study on the Neon Dimer. Journal of Chemical Theory and Computation, 2007, 3, 477-485.	5.3	15
52	Full-configuration-interaction study of the metal-insulator transition in model systems: Peierls dimerization in Hn rings and chains. Journal of Chemical Physics, 2013, 138, 074315.	3.0	15
53	Full configuration interaction calculation of singlet excited states of Be3. Journal of Chemical Physics, 2004, 121, 7103-7109.	3.0	14
54	Carbon-oxygen clusters as hypothetical high energy-density materials. Chemical Physics, 1997, 218, 21-30.	1.9	13

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55	Full Configuration-Interaction Study on the Tetrahedral Li4 Cluster. Journal of Chemical Theory and Computation, 2008, 4, 404-413.	5.3	13
56	A theoretical study of BeN linear chains: Variational and perturbative approaches. Journal of Chemical Physics, 2009, 131, 034309.	3.0	13
57	The localization tensor for the H2 molecule: Closed formulae for the Heitler-London and related wavefunctions and comparison with full configuration interaction. Journal of Chemical Physics, 2013, 138, 054314.	3.0	13
58	Electronic Bistability in Linear Beryllium Chains. Journal of Physical Chemistry A, 2009, 113, 5240-5245.	2.5	12
59	Beryllium chains interacting with Graphene Nanoislands: From anti-ferromagnetic to ferromagnetic ground state. Chemical Physics Letters, 2010, 496, 306-309.	2.6	12
60	Ab initio study of C4O4 in Td symmetry. Chemical Physics Letters, 1996, 259, 261-264.	2.6	11
61	Multi-reference configuration interaction using localized orbitals: a test study on HN. Computational and Theoretical Chemistry, 2003, 621, 51-58.	1.5	11
62	Does a Sodium Atom Bind to C60?. Journal of Chemical Theory and Computation, 2005, 1, 1079-1082.	5.3	11
63	Theoretical Study of Be_NLinear Chains: Optimized Geometries and Harmonic Frequencies. Journal of Chemical Theory and Computation, 2009, 5, 1266-1273.	5.3	11
64	Coupled-Cluster study of â€˜no-pairâ€™ bonding in the tetrahedral Cu4 cluster. Chemical Physics Letters, 2011, 503, 215-219.	2.6	11
65	Clifford Boundary Conditions: A Simple Direct-Sum Evaluation of Madelung Constants. Journal of Physical Chemistry Letters, 2020, 11, 7090-7095.	4.6	11
66	A Wigner molecule at extremely low densities: a numerically exact study. , 2019, 1, .		11
67	Application of a â€œcharge-averagedâ€•second order multireference perturbation theory strategy to the study of a model Mixed-Valence compound. Computational and Theoretical Chemistry, 2009, 896, 12-17.	1.5	10
68	Spin delocalization in hydrogen chains described with the spin-partitioned total position-spread tensor. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	10
69	Accurate ground-state energies of Wigner crystals from a simple real-space approach. Physical Review B, 2021, 103, .	3.2	10
70	Geometry optimization within a localized CAS-SCF approach. Chemical Physics Letters, 2003, 371, 49-55.	2.6	9
71	The total Position Spread in mixedâ€valence compounds: A study on the model system. Journal of Computational Chemistry, 2014, 35, 802-808.	3.3	9
72	The spin-partitioned total position-spread tensor: An application to Heisenberg spin chains. Journal of Chemical Physics, 2015, 143, 244308.	3.0	9

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73	Clifford boundary conditions for periodic systems: the Madelung constant of cubic crystals in 1, 2 and 3 dimensions. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	9
74	Effective Hamiltonians for extended systems: cyclic polyenes in the PPP approximation. Chemical Physics Letters, 1992, 196, 511-516.	2.6	8
75	An ab initio study of the N8C12 heterofullerene. International Journal of Quantum Chemistry, 1997, 65, 83-88.	2.0	8
76	Local orbitals for quasi-degenerate systems. Computational and Theoretical Chemistry, 2004, 709, 1-10.	1.5	8
77	Toward a Generalized HÃ¼ckel Rule: The Electronic Structure of Carbon Nanocones. Journal of Physical Chemistry A, 2021, 125, 9819-9825.	2.5	8
78	Surprising Electronic Structure of the BeHâ€“ Dimer: a Full-Configuration-Interaction Study. Journal of Physical Chemistry A, 2013, 117, 192-199.	2.5	7
79	The Spin-Partitioned Total-Position Spread Tensor: An Application To Diatomic Molecules. Journal of Physical Chemistry A, 2016, 120, 5230-5238.	2.5	7
80	A theoretical study on cyclacenes: Analytical tightâ€binding approach. International Journal of Quantum Chemistry, 2018, 118, e25569.	2.0	7
81	Wigner localization in two and three dimensions: An ab initio approach. Journal of Chemical Physics, 2021, 155, 124114.	3.0	7
82	Complete active-space configuration interaction with optimized orbitals: Application to Li2. International Journal of Quantum Chemistry, 1995, 55, 277-280.	2.0	6
83	Distributed Gaussian orbitals for the description of electrons in an external potential. Journal of Molecular Modeling, 2018, 24, 216.	1.8	6
84	A novel intermolecular potential to describe the interaction between the azide anion and carbon nanotubes. Diamond and Related Materials, 2020, 101, 107533.	3.9	6
85	Unique one-body position operator for periodic systems. Physical Review B, 2022, 105, .	3.2	6
86	The HÃ¼ckel Model of Polyacetylene Revisited: Asymptotic Analysis of Peierls Instability. Advances in Quantum Chemistry, 2004, 47, 347-368.	0.8	5
87	A combined freeze-and-cut strategy for the description of large molecular systems using a localized orbitals approach. Journal of Computational Chemistry, 2005, 26, 1042-1051.	3.3	5
88	Mixed Valence Character of Anionic Linear Beryllium Chains: A CAS-SCF and MR-CI Study. Journal of Physical Chemistry A, 2009, 113, 14706-14710.	2.5	5
89	A theoretical study of closed polyacene structures. Physical Chemistry Chemical Physics, 2012, 14, 15666.	2.8	5
90	A full configuration interaction study of the low-lying states of the BH molecule. Molecular Physics, 1997, 91, 861-871.	1.7	5

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91	Orbital optimization: Density matrix-based procedure versus energy minimization. Journal of Chemical Physics, 2003, 119, 11088-11094.	3.0	4
92	Possibility of a pressure-induced 2N2 ? N4 reaction. International Journal of Quantum Chemistry, 2004, 96, 598-606.	2.0	4
93	Local orbitals for excited states. Future Generation Computer Systems, 2004, 20, 821-828.	7.5	4
94	Charge transfer and mixed-valence behavior in phtalocyanine-dimer cations. Journal of Chemical Physics, 2010, 133, 124301.	3.0	4
95	The Electronic Structure of Beryllium Chains. Journal of Physical Chemistry A, 2018, 122, 5321-5332.	2.5	4
96	Spherical aromaticity and electron delocalization in $${ext{C}}_8$$ C 8 and $${ext{B}}_4{ext{N}}_4$$. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	4
97	The localization spread and polarizability of rings and periodic chains. Journal of Chemical Physics, 2021, 155, 124107.	3.0	4
98	Locality of the reduced-density-matrices: a numerical study. Chemical Physics Letters, 2004, 385, 225-230.	2.6	3
99	Computing the position-spread tensor in the CAS-SCF formalism II: Spin partition. Chemical Physics Letters, 2016, 664, 120-126.	2.6	3
100	N 3 â^' $_{3}^{-}$ azide anion confined inside finite-size carbon nanotubes. Journal of Molecular Modeling, 2017, 23, 294.	1.8	3
101	A QC collaboratory: A Grid-based Meta-System for program sharing and integration. Journal of Computational Methods in Sciences and Engineering, 2002, 2, 417-422.	0.2	2
102	A local approach to dynamical correlation. Computational and Theoretical Chemistry, 2002, 580, 39-46.	1.5	2
103	Tuning the magnetic properties of beryllium chains. Physical Chemistry Chemical Physics, 2019, 21, 6080-6086.	2.8	2
104	Distributed Gaussian orbitals for molecular calculations: application to simple systems. Molecular Physics, 2020, 118, 1615646.	1.7	2
105	Convergence of the orbital expansion in a correlated system: A test study on positronium. International Journal of Quantum Chemistry, 2001, 85, 118-126.	2.0	1
106	On the calculation of high-spin states in the full configuration-interaction formalism. Chemical Physics, 2008, 348, 83-88.	1.9	1
107	A theoretical study of saturated sp3 nitrogen rings. Computational and Theoretical Chemistry, 2008, 863, 9-15.	1.5	1
108	Cooperative modelling and design on the computing grid: data, flux and knowledge interoperability. Journal of Molecular Modeling, 2013, 19, 4215-4222.	1.8	1

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109	Confinement of the Pentanitrogen Cation Inside Carbon Nanotubes. Lecture Notes in Computer Science, 2018, , 579-592.	1.3	1
110	Extrapolation to the infinite length limit of polymer energies. I. HÃ¼ckel approximation. Journal of Chemical Physics, 1990, 92, 4383-4386.	3.0	0
111	Localized orbitals in a Multi-Reference context. Journal of Computational Methods in Sciences and Engineering, 2002, 2, 385-389.	0.2	0
112	Localized Orbitals in a Multi-Reference Context. Journal of Computational Methods in Sciences and Engineering, 2003, 3, 1-5.	0.2	0
113	Factorization of the wave-function coefficients in configuration-interaction expansions. Molecular Physics, 2005, 103, 939-947.	1.7	0