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List of Publications by Year
in descending order

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Version: 2024-02-01

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	Unique one-body position operator for periodic systems. Physical Review B, 2022, 105, .	3.2	6
2	Accurate ground-state energies of Wigner crystals from a simple real-space approach. Physical Review B, 2021, 103, .	3.2	10
3	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
4	Wigner localization in two and three dimensions: An ab initio approach. Journal of Chemical Physics, 2021, 155, 124114.	3.0	7
5	The localization spread and polarizability of rings and periodic chains. Journal of Chemical Physics, 2021, 155, 124107.	3.0	4
6	Toward a Generalized HÃ¼ckel Rule: The Electronic Structure of Carbon Nanocones. Journal of Physical Chemistry A, 2021, 125, 9819-9825.	2.5	8
7	Distributed Gaussian orbitals for molecular calculations: application to simple systems. Molecular Physics, 2020, 118, 1615646.	1.7	2
8	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
9	Clifford Boundary Conditions: A Simple Direct-Sum Evaluation of Madelung Constants. Journal of Physical Chemistry Letters, 2020, 11, 7090-7095.	4.6	11
10	A simple position operator for periodic systems. Physical Review B, 2019, 99, .	3.2	18
11	Tuning the magnetic properties of beryllium chains. Physical Chemistry Chemical Physics, 2019, 21, 6080-6086.	2.8	2
12	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
13	A Wigner molecule at extremely low densities: a numerically exact study. , 2019, 1, .		11
14	A theoretical study on cyclacenes: Analytical tightâ€binding approach. International Journal of Quantum Chemistry, 2018, 118, e25569.	2.0	7
15	Signatures of Wigner localization in one-dimensional systems. Journal of Chemical Physics, 2018, 148, 124103.	3.0	20
16	The Electronic Structure of Beryllium Chains. Journal of Physical Chemistry A, 2018, 122, 5321-5332.	2.5	4
17	Nanostructure Selectivity for Molecular Adsorption and Separation: the Case of Graphyne Layers. Journal of Physical Chemistry C, 2018, 122, 16195-16208.	3.1	32
18	Distributed Gaussian orbitals for the description of electrons in an external potential. Journal of Molecular Modeling, 2018, 24, 216.	1.8	6

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19	Confinement of the Pentanitrogen Cation Inside Carbon Nanotubes. Lecture Notes in Computer Science, 2018, , 579-592.	1.3	1
20	Increasing Radical Character of Large [n]cyclacenes Unveiled by Wave Function Theory. Journal of Physical Chemistry A, 2017, 121, 3746-3756.	2.5	45
21	N 3 â^' $_{3}^{-}$ azide anion confined inside finite-size carbon nanotubes. Journal of Molecular Modeling, 2017, 23, 294.	1.8	3
22	The Spin-Partitioned Total-Position Spread Tensor: An Application To Diatomic Molecules. Journal of Physical Chemistry A, 2016, 120, 5230-5238.	2.5	7
23	Computing the position-spread tensor in the CAS-SCF formalism II: Spin partition. Chemical Physics Letters, 2016, 664, 120-126.	2.6	3
24	The total position-spread tensor: Spin partition. Journal of Chemical Physics, 2015, 142, 094113.	3.0	16
25	The spin-partitioned total position-spread tensor: An application to Heisenberg spin chains. Journal of Chemical Physics, 2015, 143, 244308.	3.0	9
26	Spin delocalization in hydrogen chains described with the spin-partitioned total position-spread tensor. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	10
27	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
28	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
29	Computing the Position-Spread tensor in the CAS-SCF formalism. Chemical Physics Letters, 2014, 591, 58-63.	2.6	16
30	Beryllium Dimer: A Bond Based on Non-Dynamical Correlation. Journal of Physical Chemistry A, 2014, 118, 6664-6673.	2.5	44
31	Surprising Electronic Structure of the BeHâ€“ Dimer: a Full-Configuration-Interaction Study. Journal of Physical Chemistry A, 2013, 117, 192-199.	2.5	7
32	Cooperative modelling and design on the computing grid: data, flux and knowledge interoperability. Journal of Molecular Modeling, 2013, 19, 4215-4222.	1.8	1
33	Behavior of the Positionâ€“Spread Tensor in Diatomic Systems. Journal of Chemical Theory and Computation, 2013, 9, 5286-5295.	5.3	19
34	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
35	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
36	A theoretical study of closed polyacene structures. Physical Chemistry Chemical Physics, 2012, 14, 15666.	2.8	5

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37	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
38	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
39	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
40	Coupled-Cluster study of â€˜no-pairâ€™ bonding in the tetrahedral Cu4 cluster. Chemical Physics Letters, 2011, 503, 215-219.	2.6	11
41	Electron localizability and polarizability in tight-binding graphene nanostructures. Theoretical Chemistry Accounts, 2010, 126, 257-263.	1.4	19
42	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
43	Beryllium chains interacting with Graphene Nanoislands: From anti-ferromagnetic to ferromagnetic ground state. Chemical Physics Letters, 2010, 496, 306-309.	2.6	12
44	Charge transfer and mixed-valence behavior in phtalocyanine-dimer cations. Journal of Chemical Physics, 2010, 133, 124301.	3.0	4
45	Kohnâ€™s localization in the insulating state: One-dimensional lattices, crystalline versus disordered. Journal of Chemical Physics, 2010, 133, 064703.	3.0	23
46	A theoretical study of linear beryllium chains: Full configuration interaction. Journal of Chemical Physics, 2009, 130, 024301.	3.0	32
47	Abâ€initio multireference study of an organic mixedâ€valence Spiro molecular system. Journal of Computational Chemistry, 2009, 30, 83-92.	3.3	24
48	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
49	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
50	Electronic Bistability in Linear Beryllium Chains. Journal of Physical Chemistry A, 2009, 113, 5240-5245.	2.5	12
51	Theoretical Study of Be_NLinear Chains: Optimized Geometries and Harmonic Frequencies. Journal of Chemical Theory and Computation, 2009, 5, 1266-1273.	5.3	11
52	A theoretical study of BeN linear chains: Variational and perturbative approaches. Journal of Chemical Physics, 2009, 131, 034309.	3.0	13
53	End states and singletâ€“triplet degeneracy in linear atomic chains. Chemical Physics Letters, 2008, 465, 102-105.	2.6	18
54	On the calculation of high-spin states in the full configuration-interaction formalism. Chemical Physics, 2008, 348, 83-88.	1.9	1

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55	A theoretical study of saturated sp3 nitrogen rings. Computational and Theoretical Chemistry, 2008, 863, 9-15.	1.5	1
56	Full Configuration-Interaction Study on the Tetrahedral Li4 Cluster. Journal of Chemical Theory and Computation, 2008, 4, 404-413.	5.3	13
57	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
58	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
59	The metal-insulator transition in dimerized HÃ¼ckel chains. Journal of Chemical Physics, 2008, 129, 134104.	3.0	26
60	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
61	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
62	Does a Sodium Atom Bind to C60?. Journal of Chemical Theory and Computation, 2005, 1, 1079-1082.	5.3	11
63	Factorization of the wave-function coefficients in configuration-interaction expansions. Molecular Physics, 2005, 103, 939-947.	1.7	0
64	Full configuration interaction calculation of singlet excited states of Be3. Journal of Chemical Physics, 2004, 121, 7103-7109.	3.0	14
65	Full configuration interaction calculation of Be3. Journal of Chemical Physics, 2004, 120, 8405-8411.	3.0	31
66	Locality of the reduced-density-matrices: a numerical study. Chemical Physics Letters, 2004, 385, 225-230.	2.6	3
67	Possibility of a pressure-induced 2N2 ? N4 reaction. International Journal of Quantum Chemistry, 2004, 96, 598-606.	2.0	4
68	Local orbitals for excited states. Future Generation Computer Systems, 2004, 20, 821-828.	7.5	4
69	Local orbitals for quasi-degenerate systems. Computational and Theoretical Chemistry, 2004, 709, 1-10.	1.5	8
70	The HÃ¼ckel Model of Polyacetylene Revisited: Asymptotic Analysis of Peierls Instability. Advances in Quantum Chemistry, 2004, 47, 347-368.	0.8	5
71	Geometry optimization within a localized CAS-SCF approach. Chemical Physics Letters, 2003, 371, 49-55.	2.6	9
72	Localized molecular orbitals for excited states nâ†'Ï€* (CO) excitation. Chemical Physics Letters, 2003, 372, 22-27.	2.6	17

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73	Ionic nitrogen clusters. Computational and Theoretical Chemistry, 2003, 621, 43-50.	1.5	16
74	Multi-reference configuration interaction using localized orbitals: a test study on HN. Computational and Theoretical Chemistry, 2003, 621, 51-58.	1.5	11
75	Ab initio potentials for weakly interacting systems: Homonuclear rare gas dimers. International Journal of Quantum Chemistry, 2003, 95, 303-312.	2.0	20
76	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
77	The use of local orbitals in multireference calculations. Molecular Physics, 2003, 101, 1389-1398.	1.7	36
78	Multiple complete active space self-consistent field solutions. Molecular Physics, 2003, 101, 1937-1944.	1.7	22
79	Orbital optimization: Density matrix-based procedure versus energy minimization. Journal of Chemical Physics, 2003, 119, 11088-11094.	3.0	4
80	Localized Orbitals in a Multi-Reference Context. Journal of Computational Methods in Sciences and Engineering, 2003, 3, 1-5.	0.2	0
81	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
82	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
83	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
84	Localized orbitals in a Multi-Reference context. Journal of Computational Methods in Sciences and Engineering, 2002, 2, 385-389.	0.2	0
85	A local approach to dynamical correlation. Computational and Theoretical Chemistry, 2002, 580, 39-46.	1.5	2
86	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
87	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
88	Correlated description of multiple bonds using localized active orbitals. Chemical Physics Letters, 2001, 349, 555-561.	2.6	24
89	Dissociation reaction of N8 azapentalene to 4N2: A theoretical study. International Journal of Quantum Chemistry, 2000, 77, 311-315.	2.0	68
90	On the dissociation of N6 into 3 N2 molecules. Chemical Physics Letters, 2000, 320, 518-522.	2.6	47

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91	A parallel Full-CI algorithm. Computer Physics Communications, 2000, 128, 496-515.	7.5	29
92	A full-configuration benchmark for the N2 molecule. Chemical Physics Letters, 1999, 310, 530-536.	2.6	54
93	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
94	A theoretical study of ten N8 isomers. Computational and Theoretical Chemistry, 1998, 428, 1-8.	1.5	41
95	Full configuration interaction algorithm on a massively parallel architecture: Direct-list implementation. Journal of Computational Chemistry, 1998, 19, 658-672.	3.3	18
96	Ab Initio Study of Nitrogenâ^'Oxygen Clusters:Â N2O3, N4O6, and N8O12. Journal of Physical Chemistry A, 1998, 102, 4925-4929.	2.5	22
97	Is HeHâ^' a stable system?. Chemical Physics, 1997, 215, 217-225.	1.9	24
98	A theoretical study of the N 8 cubane to N 8 pentalene isomerization reaction. Theoretical Chemistry Accounts, 1997, 97, 136-142.	1.4	68
99	Carbon-oxygen clusters as hypothetical high energy-density materials. Chemical Physics, 1997, 218, 21-30.	1.9	13
100	Direct-list algorithm for configuration interaction calculations. Journal of Computational Chemistry, 1997, 18, 1329-1343.	3.3	31
101	An ab initio study of the N8C12 heterofullerene. International Journal of Quantum Chemistry, 1997, 65, 83-88.	2.0	8
102	A full configuration interaction study of the low-lying states of the BH molecule. Molecular Physics, 1997, 91, 861-871.	1.7	5
103	Ab initio study of C4O4 in Td symmetry. Chemical Physics Letters, 1996, 259, 261-264.	2.6	11
104	A one billion determinant full CI benchmark on the Cray T3D. Chemical Physics Letters, 1996, 252, 437-446.	2.6	29
105	A full CI algorithm on the CRAY T3D. Application to the NH3 molecule. Chemical Physics Letters, 1995, 233, 353-358.	2.6	27
106	Complete active-space configuration interaction with optimized orbitals: Application to Li2. International Journal of Quantum Chemistry, 1995, 55, 277-280.	2.0	6
107	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
108	Full configuration interaction calculations on Be2. Chemical Physics, 1994, 185, 47-56.	1.9	63

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109	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
110	A vector and parallel full configuration interaction algorithm. Journal of Chemical Physics, 1993, 98, 3141-3150.	3.0	108
111	Effective Hamiltonians for extended systems: cyclic polyenes in the PPP approximation. Chemical Physics Letters, 1992, 196, 511-516.	2.6	8
112	Extrapolation to the infinite length limit of polymer energies. I. HÃ¼ckel approximation. Journal of Chemical Physics, 1990, 92, 4383-4386.	3.0	0
113	Convergence of an improved CIPSI algorithm. Chemical Physics, 1983, 75, 91-102.	1.9	375