Martin SchÃ¼tz

List of Publications by Year
in descending order

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118	12,460	38660 50	23472 111
papers	citations	h-index	g-index

123	123	123	7395
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molpro: a generalâ€purpose quantum chemistry program package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 242-253.	6.2	2,852
2	Low-order scaling local electron correlation methods. I. Linear scaling local MP2. Journal of Chemical Physics, 1999, 111, 5691-5705.	1.2	671
3	Low-order scaling local electron correlation methods. IV. Linear scaling local coupled-cluster (LCCSD). Journal of Chemical Physics, 2001, 114, 661.	1.2	564
4	Density-functional theory-symmetry-adapted intermolecular perturbation theory with density fitting: A new efficient method to study intermolecular interaction energies. Journal of Chemical Physics, 2005, 122, 014103.	1.2	539
5	Low-order scaling local electron correlation methods. III. Linear scaling local perturbative triples correction (T). Journal of Chemical Physics, 2000, 113, 9986-10001.	1.2	328
6	Local perturbative triples correction (T) with linear cost scaling. Chemical Physics Letters, 2000, 318, 370-378.	1.2	296
7	High-Accuracy Computation of Reaction Barriers in Enzymes. Angewandte Chemie - International Edition, 2006, 45, 6856-6859.	7.2	253
8	An efficient local coupled cluster method for accurate thermochemistry of large systems. Journal of Chemical Physics, 2011, 135, 144116.	1.2	244
9	Local Treatment of Electron Correlation in Molecular Clusters:Â Structures and Stabilities of (H2O)n,n= 2â^'4. Journal of Physical Chemistry A, 1998, 102, 5997-6003.	1.1	231
10	Ab initio determination of the crystalline benzene lattice energy to sub-kilojoule/mole accuracy. Science, 2014, 345, 640-643.	6.0	230
11	Linear scaling local coupled cluster theory with density fitting. Part I: 4-external integrals. Physical Chemistry Chemical Physics, 2003, 5, 3349-3358.	1.3	224
12	Analytical energy gradients for local second-order MÃ¸llerâ€“Plesset perturbation theory using density fitting approximations. Journal of Chemical Physics, 2004, 121, 737-750.	1.2	220
13	Periodic local MP2 method for the study of electronic correlation in crystals: Theory and preliminary applications. Journal of Computational Chemistry, 2008, 29, 2113-2124.	1.5	216
14	Low-order scaling local correlation methods II: Splitting the Coulomb operator in linear scaling local second-order MÃ¸llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2000, 113, 9443-9455.	1.2	201
15	Intermolecular bonding and vibrations of phenolâ‹…H2O (D2O). Journal of Chemical Physics, 1993, 98, 3763-3776.	1.2	184
16	Low-order scaling local electron correlation methods. V. Connected triples beyond (T): Linear scaling local CCSDT-1b. Journal of Chemical Physics, 2002, 116, 8772-8785.	1.2	184
17	Local-MP2 electron correlation method for nonconducting crystals. Journal of Chemical Physics, 2005, 122, 094113.	1.2	182
18	Interaction Energy Contributions of H-Bonded and Stacked Structures of the AT and GC DNA Base Pairs from the Combined Density Functional Theory and Intermolecular Perturbation Theory Approach. Journal of the American Chemical Society, 2006, 128, 11730-11731.	6.6	181

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19	On the physisorption of water on graphene: a CCSD(T) study. Physical Chemistry Chemical Physics, 2011, 13, 12041.	1.3	172
20	Local CC2 electronic excitation energies for large molecules with density fitting. Journal of Chemical Physics, 2006, 125, 104106.	1.2	166
21	A new, fast, semi-direct implementation of linear scaling local coupled cluster theory. Physical Chemistry Chemical Physics, 2002, 4, 3941-3947.	1.3	164
22	The aurophilic attraction as interpreted by local correlation methods. Journal of Chemical Physics, 1999, 110, 7210-7215.	1.2	163
23	The orbital-specific-virtual local coupled cluster singles and doubles method. Journal of Chemical Physics, 2012, 136, 144105.	1.2	163
24	Fast local-MP2 method with density-fitting for crystals. I. Theory and algorithms. Physical Review B, 2007, 76, .	1.1	142
25	Fluxionality and lowâ€lying transition structures of the water trimer. Journal of Chemical Physics, 1993, 99, 5228-5238.	1.2	128
26	An ab initio derived torsional potential energy surface for (H2O)3. II. Benchmark studies and interaction energies. Journal of Chemical Physics, 1995, 103, 1085-1098.	1.2	128
27	Cryscor: a program for the post-Hartreeâ€“Fock treatment of periodic systems. Physical Chemistry Chemical Physics, 2012, 14, 7615.	1.3	122
28	The water dimer interaction energy: Convergence to the basis set limit at the correlated level. Journal of Chemical Physics, 1997, 107, 4597-4605.	1.2	115
29	A comparison of metallophilic attraction in (Xâ€“Mâ€“PH3)2 (Mâ€‰=â€‰Cu, Ag, Au; Xâ€‰=â€‰H, Cl). Physical Chemistry Chemical Physics, 2002, 4, 1006-1013.	1.3	110
30	A multistate local coupled cluster CC2 response method based on the Laplace transform. Journal of Chemical Physics, 2009, 131, 124117.	1.2	109
31	A Conclusive Mechanism of the Photoinduced Reaction Cascade in Blue Light Using Flavin Photoreceptors. Journal of the American Chemical Society, 2008, 130, 12501-12513.	6.6	103
32	Transition strengths and first-order properties of excited states from local coupled cluster CC2 response theory with density fitting. Journal of Chemical Physics, 2007, 127, 064107.	1.2	98
33	Lowâ€lying stationary points and torsional interconversions of cyclic (H2O)4: An ab initio study. Journal of Chemical Physics, 1995, 103, 6114-6126.	1.2	97
34	Fast local-MP2 method with density-fitting for crystals. II. Test calculations and application to the carbon dioxide crystal. Physical Review B, 2007, 76, .	1.1	92
35	Periodic local MÃ¸llerâ€“Plesset second order perturbation theory method applied to molecular crystals: Study of solid NH3 and CO2 using extended basis sets. Journal of Chemical Physics, 2010, 132, 134706.	1.2	81
36	The orbital-specific virtual local triples correction: OSV-L(T). Journal of Chemical Physics, 2013, 138, 054109.	1.2	81

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37	Stacking Energies for Average B-DNA Structures from the Combined Density Functional Theory and Symmetry-Adapted Perturbation Theory Approach. Journal of the American Chemical Society, 2008, 130, 1802-1803.	6.6	78
38	Correlation regions within a localized molecular orbital approach. Journal of Chemical Physics, 2008, 128, 144106.	1.2	76
39	Integral-direct electron correlation methods. Molecular Physics, 1999, 96, 719-733.	0.8	75
40	Benzyne Thermochemistry:Â A Benchmark ab Initio Study. Journal of Physical Chemistry A, 1999, 103, 9913-9920.	1.1	75
41	Experimental and Theoretical Studies of the d8â^'d10Interaction between Pd(II) and Au(I):Â Bis(chloro[(phenylthiomethyl)diphenylphosphine]gold(I))â^'dichloropalladium(II) and Related Systems. Inorganic Chemistry, 2000, 39, 4786-4792.	1.9	75
42	Local CC2 response method for triplet states based on Laplace transform: Excitation energies and first-order properties. Journal of Chemical Physics, 2010, 133, 244110.	1.2	66
43	Structures and vibrations of phenol Â· H2O and d-phenol Â· D2O based on ab initio calculations. Computational and Theoretical Chemistry, 1992, 276, 117-132.	1.5	64
44	Theoretical Study on the Repair Mechanism of the (6â^'4) Photolesion by the (6â^'4) Photolyase. Journal of the American Chemical Society, 2010, 132, 16285-16295.	6.6	63
45	Toward an Accurate Estimate of the Exfoliation Energy of Black Phosphorus: A Periodic Quantum Chemical Approach. Journal of Physical Chemistry Letters, 2016, 7, 131-136.	2.1	62
46	Intermolecular vibrations of phenolâ‹…(H2O)3 and d1â€phenolâ‹…(D2O)3 in the S0 and S1 states. Journal of Chemical Physics, 1995, 103, 6350-6361.	1.2	61
47	On the use of the Laplace transform in local correlation methods. Physical Chemistry Chemical Physics, 2008, 10, 3430.	1.3	54
48	Two-dimensional model treatment of torsional motions in the water trimer. Chemical Physics Letters, 1995, 237, 536-544.	1.2	53
49	Second Order Local MÃ¸ller-Plesset Perturbation Theory for Periodic Systems: the CRYSCOR Code. Zeitschrift Fur Physikalische Chemie, 2010, 224, 441-454.	1.4	52
50	Improved intermolecular water potential from global geometry optimization of small water clusters using local MP2. Chemical Physics, 1998, 239, 561-572.	0.9	51
51	Approaching the theoretical limit in periodic local MP2 calculations with atomic-orbital basis sets: The case of LiH. Journal of Chemical Physics, 2011, 134, 214105.	1.2	49
52	Intermolecular bonding and vibrations of 2â€naphtholâ‹…H2O (D2O). Journal of Chemical Physics, 1993, 99, 1469-1481.	1.2	44
53	MP2 versus density-functional theory study of the Compton profiles of crystalline urea. Physical Review B, 2010, 81, .	1.1	43
54	Periodic local MP2 method employing orbital specific virtuals. Journal of Chemical Physics, 2015, 143, 102805.	1.2	43

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55	Singlet benzyne thermochemistry: a CASPT2 study of the enthalpies of formation. Chemical Physics Letters, 1996, 258, 409-415.	1.2	42
56	Efficient and accurate treatment of weak pairs in local CCSD(T) calculations. Journal of Chemical Physics, 2013, 139, 164116.	1.2	42
57	Efficient and accurate treatment of weak pairs in local CCSD(T) calculations. II. Beyond the ring approximation. Journal of Chemical Physics, 2014, 140, 244107.	1.2	42
58	Local CC2 response method based on the Laplace transform: Analytic energy gradients for ground and excited states. Journal of Chemical Physics, 2014, 140, 164113.	1.2	39
59	NMR shielding tensors for density fitted local second-order MÃ¸ller-Plesset perturbation theory using gauge including atomic orbitals. Journal of Chemical Physics, 2012, 137, 084107.	1.2	37
60	The Mechanism of Spectral Shift and Inhomogeneous Broadening of an Aromatic Chromophore in a Polymer Glass. Journal of the American Chemical Society, 1995, 117, 7493-7507.	6.6	36
61	A QM/MM study on the fast photocycle of blue light using flavin photoreceptors in their light-adapted/active form. Physical Chemistry Chemical Physics, 2010, 12, 8840.	1.3	36
62	Periodic and fragment models based on the local correlation approach. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1357.	6.2	36
63	A comparison between quantum chemistry and quantum Monte Carlo techniques for the adsorption of water on the (001) LiH surface. Journal of Chemical Physics, 2017, 146, 204108.	1.2	35
64	Force-constant weighted redundant coordinates in molecular geometry optimizations. Chemical Physics Letters, 1999, 303, 567-575.	1.2	34
65	Periodic quantum mechanical simulation of the Heâ€“MgO(100) interaction potential. Journal of Chemical Physics, 2011, 134, 014706.	1.2	34
66	The molecular and electronic structure ofsâ€tetrazine in the ground and first excited state: A theoretical investigation. Journal of Chemical Physics, 1995, 103, 7048-7057.	1.2	33
67	Exfoliation Energy of Black Phosphorus Revisited: A Coupled Cluster Benchmark. Journal of Physical Chemistry Letters, 2017, 8, 1290-1294.	2.1	33
68	Geometrical frustration of an argon monolayer adsorbed on the MgO (100) surface: An accurate periodicab initiostudy. Physical Review B, 2012, 86, .	1.1	31
69	The ammonia dimer equilibrium dissociation energy: convergence to the basis set limit at the correlated level. Molecular Physics, 2002, 100, 3389-3399.	0.8	30
70	On the Photophysics of Artificial Blue-Light Photoreceptors:Â An Ab Initio Study on a Flavin-Based Dye Dyad at the Level of Coupled-Cluster Response Theory. Journal of the American Chemical Society, 2007, 129, 4068-4074.	6.6	30
71	Application of Hermitian time-dependent coupled-cluster responseAnsÃtzeof second order to excitation energies and frequency-dependent dipole polarizabilities. Physical Review A, 2012, 86, .	1.0	28
72	Ab Initio Calculations of the Binding Energies of Small (H₂O)_n Clusters (n =) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.9	27

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73	Helical Chirality in Pentacoordinate Zinc Complexes-Selective Access to Both Pseudoenantiomers with One Ligand Configuration. Angewandte Chemie - International Edition, 2005, 44, 242-245.	7.2	27
74	Local Approximations for an Efficient and Accurate Treatment of Electron Correlation and Electron Excitations in Molecules. Challenges and Advances in Computational Chemistry and Physics, 2011, , 345-407.	0.6	27
75	On the significance of the trigger reaction in the action of the calicheamicin ? 1 I anti-cancer drug. Theoretical Chemistry Accounts, 1997, 97, 203-210.	0.5	25
76	Electron correlation decides the stability of cubic versus hexagonal boron nitride. Physical Review B, 2011, 83, .	1.1	25
77	Structures, dynamics and vibrations of cyclic (H2O)3and its phenyl and naphthyl derivatives. Faraday Discussions, 1994, 97, 285-297.	1.6	24
78	Local Time-Dependent Coupled Cluster Response for Properties of Excited States in Large Molecules. Zeitschrift Fur Physikalische Chemie, 2010, 224, 601-616.	1.4	24
79	Local ab initio methods for calculating optical band gaps in periodic systems. I. Periodic density fitted local configuration interaction singles method for polymers. Journal of Chemical Physics, 2011, 134, 094101.	1.2	24
80	Density fitted, local Hartreeâ€“Fock treatment of NMR chemical shifts using London atomic orbitals. Molecular Physics, 2010, 108, 477-485.	0.8	23
81	Local CC2 response method based on the Laplace transform: Orbital-relaxed first-order properties for excited states. Journal of Chemical Physics, 2013, 139, 084111.	1.2	23
82	An integral direct, distributed-data, parallel MP2 algorithm. Theoretica Chimica Acta, 1997, 95, 13.	0.9	22
83	Oscillator strengths, first-order properties, and nuclear gradients for local ADC(2). Journal of Chemical Physics, 2015, 142, 214103.	1.2	21
84	Molecular aniline clusters. I. The electronic ground state. Journal of Chemical Physics, 2010, 132, 174303.	1.2	19
85	Second-order variational coupled-cluster linear-response method: A Hermitian time-dependent theory. Physical Review A, 2011, 83, .	1.0	19
86	Fragment-Based Direct-Local-Ring-Coupled-Cluster Doubles Treatment Embedded in the Periodic Hartreeâ€“Fock Solution. Journal of Chemical Theory and Computation, 2016, 12, 5145-5156.	2.3	19
87	Nb and Ta Adducts: Connecting d⁰ Metal Chlorides and Phosphorus Sulfide Cages. Chemistry - A European Journal, 2009, 15, 7129-7138.	1.7	17
88	Approaching an exact treatment of electronic correlations at solid surfaces: The binding energy of the lowest bound state of helium adsorbed on MgO(100). Physical Review B, 2014, 89, .	1.1	17
89	An integral direct, distributed-data, parallel MP2 algorithm. Theoretica Chimica Acta, 1997, 95, 13-34.	0.9	16
90	Why BLUF photoreceptors with roseoflavincofactors lose their biological functionality. Physical Chemistry Chemical Physics, 2011, 13, 14775.	1.3	16

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91	Orbital-unrelaxed Lagrangian density matrices for periodic systems at the local MP2 level. Journal of Physics: Conference Series, 2008, 117, 012027.	0.3	15
92	Comment on â€œMinimax approximation for the decomposition of energy denominators in Laplace-transformed MÃ¸llerâ€“Plesset perturbation theoriesâ€•[J. Chem. Phys. 129, 044112 (2008)]. Journal of Chemical Physics, 2009, 130, 127101.	1.2	15
93	A hierarchy of local coupled cluster singles and doubles response methods for ionization potentials. Journal of Chemical Physics, 2016, 144, 084117.	1.2	15
94	On the exfoliation and anisotropic thermal expansion of black phosphorus. Chemical Communications, 2018, 54, 9793-9796.	2.2	15
95	Local ab initio methods for calculating optical bandgaps in periodic systems. II. Periodic density fitted local configuration interaction singles method for solids. Journal of Chemical Physics, 2012, 137, 204119.	1.2	14
96	Phenol-water1â©½nâ©½3 revisited: An ab initio study on the photophysics of these clusters at the level of coupled cluster response theory. Journal of Chemical Physics, 2007, 127, 174304.	1.2	13
97	A comparison between the NEMO intermolecular water potential and ab initio quantum chemical calculations for the water trimer and tetramer. Molecular Physics, 1997, 90, 277-287.	0.8	13
98	Conformational control of benzophenone-sensitized charge transfer in dinucleotides. Physical Chemistry Chemical Physics, 2013, 15, 18607.	1.3	12
99	Nonorthogonal ultralocalized functions and fitted Wannier functions for local electron correlation methods for solids. Theoretical Chemistry Accounts, 2005, 114, 276-282.	0.5	11
100	The 2-naphthol-water2 cluster: Two competing types of hydrogen-bonding arrangements. Journal of Chemical Physics, 2008, 129, 034301.	1.2	11
101	Molecular aniline clusters. II. The low-lying electronic excited states. Journal of Chemical Physics, 2010, 133, 134307.	1.2	11
102	He-atom scattering from MgO(100): calculating diffraction peak intensities with a semi ab initio potential. Physical Chemistry Chemical Physics, 2011, 13, 14750.	1.3	11
103	Magnetizability and rotational g tensors for density fitted local second-order MÃ¸ller-Plesset perturbation theory using gauge-including atomic orbitals. Journal of Chemical Physics, 2014, 141, 024108.	1.2	11
104	Diffraction of helium on MgO(100) surface calculated from first-principles. Physical Chemistry Chemical Physics, 2014, 16, 21106-21113.	1.3	11
105	Integral-direct electron correlation methods. , 0, .		11
106	A comparison between the NEMO intermolecular water potential and ab initio quantum chemical calculations for the water trimer tetramer. Molecular Physics, 1997, 90, 277-287.	0.8	8
107	Semidirect parallel self-consistent field: the load balancing problem in the input/output intensive self-consistent field iterations. Theoretical Chemistry Accounts, 2003, 110, 156-164.	0.5	8
108	Intermolecular Interactions in Photodamaged DNA from Density Functional Theory Symmetryâ€Adapted Perturbation Theory. ChemPhysChem, 2011, 12, 1251-1254.	1.0	7

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109	Dispersion interactions in silicon allotropes. Physical Chemistry Chemical Physics, 2017, 19, 7699-7707.	1.3	7
110	Phase transition in GeF<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>driven by change of type of intermolecular interaction. Physical Review B, 2012, 86, .	1.1	5
111	Heterogeneous Clusters of Phthalocyanine and Water Prepared and Probed in Superfluid Helium Nanodroplets. Journal of Physical Chemistry A, 2019, 123, 10057-10064.	1.1	4
112	Influencing the conductance in biphenylâ€like molecular junctions with THz radiation. Physica Status Solidi (B): Basic Research, 2013, 250, 2408-2416.	0.7	3
113	14 Description of excited states in photocatalysis with theoretical methods. , 2013, , 263-294.		2
114	Description of excited states in photochemistry with theoretical methods. ChemistrySelect, 2021, 6, .	0.7	2
115	Theoretische Chemie 2002. Nachrichten Aus Der Chemie, 2003, 51, 323-329.	0.0	0
116	Inside Cover: Intermolecular Interactions in Photodamaged DNA from Density Functional Theory Symmetryâ€Adapted Perturbation Theory (ChemPhysChem 7/2011). ChemPhysChem, 2011, 12, 1206-1206.	1.0	0
117	16. Description of excited states in photochemistry with theoretical methods. , 2020, , 379-414.		0
118	Second Order Local Mller-Plesset Perturbation Theory for Periodic Systems: the CRYSCOR Code. , 2010, , 151-164.		0