Andreas KÃ¶hn

List of Publications by Year
in descending order

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80	6,928	87888 38	62596 80
papers	citations	h-index	g-index

81	81	81	5199
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Adsorption Geometries and Electronic Properties of a Dipolar Phosphonate-Based Monolayer on the NiO Surface. Journal of Physical Chemistry C, 2022, 126, 5793-5804.	3.1	1
2	Thermally Averaged Magnetic Anisotropy Tensors via Machine Learning Based on Gaussian Moments. Journal of Chemical Theory and Computation, 2022, 18, 1-12.	5.3	10
3	Towards photoassociation processes of ultracold rubidium trimers. Physical Review A, 2021, 103, .	2.5	8
4	On the Accuracy of Mean-Field Spinâ€“Orbit Operators for 3d Transition-Metal Systems. Journal of Chemical Theory and Computation, 2021, 17, 5530-5537.	5.3	6
5	Limitations of perturbative coupled-cluster approximations for highly accurate investigations of Rb2+. Journal of Chemical Physics, 2021, 155, 124101.	3.0	1
6	A generalized hybrid scheme for multireference methods. Journal of Chemical Physics, 2021, 155, 204106.	3.0	1
7	Improved and simplified orthogonalisation scheme and connected triples correction within the internally contracted multireference coupled-cluster method. Molecular Physics, 2020, 118, e1743889.	1.7	6
8	The Molpro quantum chemistry package. Journal of Chemical Physics, 2020, 152, 144107.	3.0	603
9	Liquid Crystalline Benzoic Acid Ester MIDA Boronates: Synthesis and Mesomorphic Properties. Organic Materials, 2020, 02, 288-299.	2.0	2
10	The second-order approximate internally contracted multireference coupled-cluster singles and doubles method icMRCC2. Journal of Chemical Physics, 2019, 151, 041106.	3.0	10
11	Linear and quadratic internally contracted multireference coupled-cluster approximations. Journal of Chemical Physics, 2019, 150, 194107.	3.0	9
12	The extended explicitly-correlated second-order approximate coupled-cluster singles and doubles ansatz suitable for response theory. Journal of Chemical Physics, 2019, 150, 184110.	3.0	3
13	On the distinguishable cluster approximation for triple excitations. Journal of Chemical Physics, 2019, 150, 151101.	3.0	17
14	Perturbation Expansion of Internally Contracted Coupled-Cluster Theory up to Third Order. Journal of Chemical Theory and Computation, 2019, 15, 2291-2305.	5.3	14
15	Embedded Multireference Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2018, 14, 693-709.	5.3	30
16	Origin of the Ï€â€“Ï€ Spacing Change upon Doping of Semiconducting Polymers. Journal of Physical Chemistry C, 2018, 122, 27983-27990.	3.1	25
17	A model hamiltonian tuned toward high level ab initio calculations to describe the character of excitonic states in perylenebisimide aggregates. Journal of Computational Chemistry, 2018, 39, 1979-1989.	3.3	14
18	Do CCSD and approximate CCSD-F12 variants converge to the same basis set limits? The case of atomization energies. Journal of Chemical Physics, 2018, 149, 154109.	3.0	48

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19	First-order properties from internally contracted multireference coupled-cluster theory with particular focus on hyperfine coupling tensors. Journal of Chemical Physics, 2018, 149, 064101.	3.0	9
20	Internally Contracted Multireference Coupled Cluster Calculations with a Spin-Free Diracâ€“Coulomb Hamiltonian: Application to the Monoxides of Titanium, Zirconium, and Hafnium. Journal of Chemical Theory and Computation, 2017, 13, 3171-3184.	5.3	7
21	How To Arrive at Accurate Benchmark Values for Transition Metal Compounds: Computation or Experiment?. Journal of Chemical Theory and Computation, 2017, 13, 5291-5316.	5.3	101
22	Surface hopping dynamics including intersystem crossing using the algebraic diagrammatic construction method. Journal of Chemical Physics, 2017, 147, 184109.	3.0	32
23	Doping mechanism of MoO₃in 4,4â€²-Bis(N-carbazolyl)-1,1â€²-biphenyl: A photoelectron spectroscopic study. Physica Status Solidi (B): Basic Research, 2016, 253, 1697-1706.	1.5	7
24	Quantum tunneling during interstellar surface-catalyzed formation of water: the reaction H + H₂O₂ â†’ H₂O + OH. Physical Chemistry Chemical Physics, 2016, 18, 33021-33030.	2.8	36
25	Internally contracted multireference coupled-cluster theory in a multistate framework. Journal of Chemical Physics, 2016, 144, 074103.	3.0	25
26	Revisiting the F + HCl â†’ HF + Cl reaction using a multireference coupled-cluster method. Physical Chemistry Chemical Physics, 2016, 18, 30241-30253.	2.8	12
27	Synthesis of the AB ring system of clifednamide utilizing Claisen rearrangement and Dielsâ€“Alder reaction as key steps. Organic and Biomolecular Chemistry, 2016, 14, 884-894.	2.8	8
28	A general ansatz for constructing quasi-diabatic states in electronically excited aggregated systems. Journal of Chemical Physics, 2015, 143, 084106.	3.0	30
29	Intramolecular Charge-Transfer Excited-State Processes in 4-(N,N-Dimethylamino)benzonitrile: The Role of Twisting and the ï€ï*ƒ* State. Journal of Physical Chemistry A, 2015, 119, 6232-6243.	2.5	60
30	Excited states with internally contracted multireference coupled-cluster linear response theory. Journal of Chemical Physics, 2014, 140, 134108.	3.0	39
31	Emergence of Coherence through Variation of Intermolecular Distances in a Series of Molecular Dimers. Journal of Physical Chemistry Letters, 2014, 5, 262-269.	4.6	37
32	Stateâ€specific multireference coupledâ€cluster theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 176-197.	14.6	98
33	Solvent Effects on Electronically Excited States Using the Conductor-Like Screening Model and the Second-Order Correlated Method ADC(2). Journal of Chemical Theory and Computation, 2013, 9, 977-994.	5.3	119
34	Infrared study of the MoO3 doping efficiency in 4,4â€²-bis(N-carbazolyl)-1,1â€²-biphenyl (CBP). Organic Electronics, 2013, 14, 575-583.	2.6	52
35	Explicitly correlated internally contracted multireference coupled-cluster singles and doubles theory: ic-MRCCSD(F12â^—). Chemical Physics Letters, 2013, 565, 122-127.	2.6	25
36	A sequential transformation approach to the internally contracted multireference coupled cluster method. Journal of Chemical Physics, 2012, 136, 204108.	3.0	56

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37	Perturbative treatment of triple excitations in internally contracted multireference coupled cluster theory. Journal of Chemical Physics, 2012, 136, 204107.	3.0	79
38	Quantum Chemical Parametrization and Spectroscopic Characterization of the Frenkel Exciton Hamiltonian for a J-Aggregate Forming Perylene Bisimide Dye. Journal of Physical Chemistry A, 2012, 116, 11451-11458.	2.5	41
39	Communication: Restoring full size extensivity in internally contracted multireference coupled cluster theory. Journal of Chemical Physics, 2012, 137, 131103.	3.0	56
40	Ab Initio Studies of Triplet-State Properties for Organic Semiconductor Molecules. Journal of Physical Chemistry C, 2012, 116, 15203-15217.	3.1	20
41	Kommentar zu: H. Mustroph, S. Ernst â€œDas Franck-Condon-Prinzipâ€: Chemie in Unserer Zeit, 2012, 46, 117-118.	0.1	1
42	Explicitly Correlated Electrons in Molecules. Chemical Reviews, 2012, 112, 4-74.	47.7	487
43	Meaning and magnitude of the reduced density matrix cumulants. Chemical Physics, 2012, 401, 50-61.	1.9	38
44	The Triplet Excimer of Naphthalene: A Model System for Tripletâ^'Triplet Interactions and Its Spectral Properties. Journal of Physical Chemistry C, 2011, 115, 8335-8344.	3.1	34
45	Pilot applications of internally contracted multireference coupled cluster theory, and how to choose the cluster operator properly. Journal of Chemical Physics, 2011, 134, 204111.	3.0	156
46	A worrisome failure of the CC2 coupled-cluster method when applied to ozone. Chemical Physics Letters, 2010, 495, 135-140.	2.6	30
47	Towards the Hartreeâ€“Fock and coupled-cluster singles and doubles basis set limit: A study of various models that employ single excitations into a complementary auxiliary basis set. Journal of Chemical Physics, 2010, 132, 024101.	3.0	29
48	Communications: Accurate and efficient approximations to explicitly correlated coupled-cluster singles and doubles, CCSD-F12. Journal of Chemical Physics, 2010, 132, 231102.	3.0	259
49	Explicitly correlated coupled-cluster theory using cusp conditions. I. Perturbation analysis of coupled-cluster singles and doubles (CCSD-F12). Journal of Chemical Physics, 2010, 133, 174117.	3.0	38
50	Explicitly correlated coupled-cluster theory using cusp conditions. II. Treatment of connected triple excitations. Journal of Chemical Physics, 2010, 133, 174118.	3.0	44
51	Excited States of [3.3](4,4â€²)Biphenylophane: The Role of Charge-Transfer Excitations in Dimers With Ï€â^'Ï€ Interaction. Journal of Physical Chemistry A, 2010, 114, 1639-1649.	2.5	15
52	Combined Experimental and Theoretical Study of the Vibronic Spectra of Perylenecarboximides. Journal of Physical Chemistry B, 2010, 114, 1638-1647.	2.6	21
53	A modified ansatz for explicitly correlated coupled-cluster wave functions that is suitable for response theory. Journal of Chemical Physics, 2009, 130, 104104.	3.0	53
54	Response properties with explicitly correlated coupled-cluster methods using a Slater-type correlation factor and cusp conditions. Journal of Chemical Physics, 2009, 131, 124118.	3.0	45

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55	Explicitly correlated connected triple excitations in coupled-cluster theory. Journal of Chemical Physics, 2009, 130, 131101.	3.0	82
56	FÃ¶rster Energy Transfer and Davydov Splittings in Time-Dependent Density Functional Theory: Lessons from 2-Pyridone Dimer. Journal of Chemical Theory and Computation, 2009, 5, 873-880.	5.3	32
57	Theoretical investigation of electronic excitation energy transfer in bichromophoric assemblies. Journal of Chemical Physics, 2008, 128, 074505.	3.0	84
58	Implementation of transition moments between excited states in the approximate coupled-cluster singles and doubles model. Journal of Chemical Physics, 2008, 129, 214101.	3.0	47
59	Implementation of the full explicitly correlated coupled-cluster singles and doubles model CCSD-F12 with optimally reduced auxiliary basis dependence. Journal of Chemical Physics, 2008, 129, 201103.	3.0	86
60	Can coupled-cluster theory treat conical intersections?. Journal of Chemical Physics, 2007, 127, 044105.	3.0	81
61	Distributed memory parallel implementation of energies and gradients for second-order MÃ¸llerâ€“Plesset perturbation theory with the resolution-of-the-identity approximation. Physical Chemistry Chemical Physics, 2006, 8, 1159.	2.8	223
62	Intramolecular Charge-Transfer Mechanism in Quinolidines:Â The Role of the Amino Twist Angle. Journal of the American Chemical Society, 2006, 128, 15672-15682.	13.7	54
63	The First End-On Bonded Superoxo Complexes of Ga and In: The Oxygen-Rich Compounds GaO4 and InO4. European Journal of Inorganic Chemistry, 2006, 2006, 1496-1504.	2.0	10
64	High-order correlation effects on dynamic hyperpolarizabilities and their geometric derivatives: A comparison with density functional results. Journal of Chemical Physics, 2006, 124, 114101.	3.0	46
65	Coupled-cluster with active space selected higher amplitudes: Performance of seminatural orbitals for ground and excited state calculations. Journal of Chemical Physics, 2006, 125, 174110.	3.0	40
66	On the Oxidation of Gallium and Indium: Characterization of the Cyclic and Linear GaO2 and InO2 Molecules Generated by the Spontaneous and Photoinduced Reaction of Ga and In Atoms with O2 and Determination of the Reaction Mechanism. Chemistry - A European Journal, 2005, 11, 5575-5588.	3.3	15
67	Frequency-dependent hyperpolarizabilities of the Ne, Ar, and Kr atoms using the approximate coupled cluster triples model CC3. Journal of Chemical Physics, 2005, 123, 094303.	3.0	12
68	The trust-region self-consistent field method in Kohnâ€“Sham density-functional theory. Journal of Chemical Physics, 2005, 123, 074103.	3.0	31
69	Orbital-optimized coupled-cluster theory does not reproduce the full configuration-interaction limit. Journal of Chemical Physics, 2005, 122, 084116.	3.0	52
70	On the Nature of the Low-Lying Singlet States of 4-(Dimethyl-amino)benzonitrile. Journal of the American Chemical Society, 2004, 126, 7399-7410.	13.7	113
71	Ab Initio Calculation of the Vibrational and Electronic Spectra of trans- and cis-Azobenzene. Journal of the American Chemical Society, 2003, 125, 9821-9827.	13.7	194
72	Why Does a Ga2 Dimer React Spontaneously with H2, but a Ga Atom Does Not?â€”A Detailed Quantum Chemical Investigation of the Differences in Reactivity Between Ga Atoms and Ga2 Dimers, in Combination with Experimental Results. Chemistry - A European Journal, 2003, 9, 3909-3919.	3.3	49

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73	Analytic gradients for excited states in the coupled-cluster model CC2 employing the resolution-of-the-identity approximation. Journal of Chemical Physics, 2003, 119, 5021-5036.	3.0	372
74	Transition moments and excited-state first-order properties in the coupled-cluster model CC2 using the resolution-of-the-identity approximation. Journal of Chemical Physics, 2002, 117, 6939-6951.	3.0	402
75	First-order properties for triplet excited states in the approximated coupled cluster model CC2 using an explicitly spin coupled basis. Journal of Chemical Physics, 2002, 116, 5401-5410.	3.0	60
76	Efficient use of the correlation consistent basis sets in resolution of the identity MP2 calculations. Journal of Chemical Physics, 2002, 116, 3175-3183.	3.0	1,671
77	Comment on `Efficient calculation of canonical MP2 energies' [P. Pulay, S. SaebÃ¸, K. Wolinski, Chem. Phys. Lett. 344 (2001) 543â€“552]. Chemical Physics Letters, 2002, 358, 350-353.	2.6	5
78	Theoretical study on clusters of magnesium. Physical Chemistry Chemical Physics, 2001, 3, 711-719.	2.8	122
79	Photodissociation spectroscopy of Ag[sub 4][sup +](N[sub 2])[sub m], m=0â€“4. Journal of Chemical Physics, 2000, 113, 5361.	3.0	36
80	Chasing polycyclic natural products: 5/6/5â€•or 5/6/6â€•carbotricyclic scaffold construction via stereodivergent Dielsâ€Alder reaction of chiral hydrindanes and their boron complexes. European Journal of Organic Chemistry, 0, , .	2.4	0