Priv-Dozâ€Dr Dirk Andrae

List of Publications by Year
in descending order

45 papers	8,374 citations	586496 16 h-index	299063 42 g-index
48 all docs	48 docs citations	48 times ranked	9395 citing authors

#	Article	IF	Citations
1	Searching for Monomeric Nickel Tetrafluoride: Unravelling Infrared Matrix Isolation Spectra of Higher Nickel Fluorides. Angewandte Chemie, 2021, 133, 6461-6464.	1.6	5
2	Searching for Monomeric Nickel Tetrafluoride: Unravelling Infrared Matrix Isolation Spectra of Higher Nickel Fluorides. Angewandte Chemie - International Edition, 2021, 60, 6391-6394.	7.2	12
3	Molecular oxofluorides OMFn of nickel, palladium and platinum: oxyl radicals with moderate ligand field inversion. Inorganic Chemistry Frontiers, 2021, 8, 1215-1228.	3.0	11
4	Local Orbitals in Quantum Chemistry. Lecture Notes in Quantum Chemistry II, 2021, , 41-101.	0.3	2
5	Analytical solutions for the diffusive mass transfer at cylindrical and hollow-cylindrical electrodes with reflective and transmissive boundary conditions. Journal of Electroanalytical Chemistry, 2021, 897, 115565.	1.9	2
6	Universal Algorithm for Simulating and Evaluating Cyclic Voltammetry at Macroporous Electrodes by Considering Random Arrays of Microelectrodes. ChemPhysChem, 2020, 21, 428-441.	1.0	18
7	Real-space simulation of cyclic voltammetry in carbon felt electrodes by combining micro X-ray CT data, digital simulation and convolutive modeling. Electrochimica Acta, 2020, 353, 136487.	2.6	6
8	Low-lying electronic terms of diatomic molecules AB (A = Scâ€“Ni, B = Cu/Ag/Au). Molecular Physics, 2020, 118, e1772514.	0.8	2
9	Theory of cyclic voltammetry in random arrays of cylindrical microelectrodes applied to carbon felt electrodes for vanadium redox flow batteries. Physical Chemistry Chemical Physics, 2019, 21, 9061-9068.	1.3	28
10	Oxygen radical character in group 11 oxygen fluorides. Nature Communications, 2018, 9, 1267.	5.8	11
11	Increasing Radical Character of Large [n]cyclacenes Unveiled by Wave Function Theory. Journal of Physical Chemistry A, 2017, 121, 3746-3756.	1.1	45
12	A computational study of samarium diiodideâ€induced cyclizations of Nâ€oxoalkylâ€substituted methyl indoleâ€3â€carboxylatesâ€”A rationale of the diastereoselectivity. Journal of Computational Chemistry, 2017, 38, 2693-2700.	1.5	5
13	Wissenschaftliche StammbÃume der theoretischen Chemie. Nachrichten Aus Der Chemie, 2017, 65, 1137-1140.	0.0	0
14	Nuclear Charge Density and Magnetization Distributions. , 2017, , 51-81.		3
15	Low-Lying Electronic States of CuAu. Journal of Physical Chemistry A, 2016, 120, 5856-5867.	1.1	2
16	Static electric dipole polarizabilities for isoelectronic sequences. II. Open-shell S states. European Physical Journal D, 2013, 67, 1.	0.6	5
17	Electronic Origin of the Structural Anomalies of Zinc and Cadmium. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 2036-2046.	0.6	8
18	A Firstâ€Principles Study of Electronic Structure of the Laves Phase MgZn₂. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 1963-1967.	0.6	8

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19	Fast and accurate 3D tensor calculation of the Fock operator in a general basis. Computer Physics Communications, 2012, 183, 2392-2404.	3.0	17
20	Low-temperature formation of cubic Î²-PbF2: precursor-based synthesis and first-principles phase stability study. Physical Chemistry Chemical Physics, 2011, 13, 6029.	1.3	5
21	Electronic Quantum Fluxes during Pericyclic Reactions Exemplified for the Cope Rearrangement of Semibullvalene. Journal of Physical Chemistry B, 2011, 115, 5476-5483.	1.2	46
22	Static electric dipole polarizabilities for isoelectronic sequences. International Journal of Quantum Chemistry, 2011, 111, 891-903.	1.0	11
23	An empirical formula to estimate off-diagonal adiabatic corrections to rotationâ€“vibrational energy levels. Theoretical Chemistry Accounts, 2010, 127, 149-155.	0.5	8
24	Understanding the hcp anisotropy in Cd and Zn: the role of electron correlation in determining the potential energy surface. Physical Chemistry Chemical Physics, 2010, 12, 681-687.	1.3	25
25	A Theoretical Study of Polyoxometalates andÂDendrizyme Model Compounds. , 2009, , 129-142.		1
26	Molecular Dynamics Simulations of Dendrimer-Encapsulated Î±-Keggin Ions in Trichloromethane Solution. Journal of Physical Chemistry B, 2008, 112, 5153-5162.	1.2	23
27	Molecular knots, links, and fabrics: prediction of existence and suggestion of a synthetic route. New Journal of Chemistry, 2006, 30, 873.	1.4	22
28	Discrete contributions to static dipole polarizabilities of excited bound states of non-relativistic hydrogen-like atoms. Theoretical Chemistry Accounts, 2005, 114, 380-386.	0.5	2
29	Asymptotically exact calculation of the exchange energies of one-active-electron diatomic ions with the surface integral method. Journal of Physics B: Atomic, Molecular and Optical Physics, 2004, 37, 4451-4469.	0.6	8
30	Exchange Energy for Two-Active-Electron Diatomic Systems Within the Surface Integral Method. Applicable Algebra in Engineering, Communications and Computing, 2004, 15, 101.	0.3	2
31	Chapter 4 Nuclear charge density distributions in quantum chemistry. Theoretical and Computational Chemistry, 2002, 11, 203-258.	0.2	7
32	Asymptotics of Quantum Mechanical Atom-Ion Systems. Applicable Algebra in Engineering, Communications and Computing, 2002, 13, 233-255.	0.3	5
33	Numerical self-consistent field method for polyatomic molecules. Molecular Physics, 2001, 99, 327-334.	0.8	14
34	Examination of several density functionals in numerical Kohn-Sham calculations for atoms. International Journal of Quantum Chemistry, 2001, 82, 227-241.	1.0	11
35	Numerical electronic structure calculations for atoms. II. Generalized variable transformation and relativistic calculations. International Journal of Quantum Chemistry, 2000, 76, 473-499.	1.0	19
36	Finite nuclear charge density distributions in electronic structure calculations for atoms and molecules. Physics Reports, 2000, 336, 413-525.	10.3	107

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37	A comparative study of finite nucleus models for low-lying states of few-electron high-Z atoms. Chemical Physics Letters, 2000, 320, 457-468.	1.2	17
38	Recursive evaluation of expectation values for arbitrary states of the relativistic one-electron atom. Journal of Physics B: Atomic, Molecular and Optical Physics, 1997, 30, 4435-4451.	0.6	30
39	Numerical electronic structure calculations for atoms. I. Generalized variable transformation and nonrelativistic calculations. International Journal of Quantum Chemistry, 1997, 63, 65-91.	1.0	29
40	Comment on â€œcomparison of the widely used HF pseudo-potentials: MH+ (M = Fe, Ru, Os)â€• Chemical Physics Letters, 1994, 220, 341-344.	1.2	8
41	Comparison of Spectroscopic Constants of OsH from Different ab Initio Calculations. Journal of Molecular Spectroscopy, 1993, 160, 585-589.	0.4	2
42	Comment on â€œspectroscopic constants and potential energy curves of OsHâ€•by M. Benavides-Garcia and K. Balasubramanian. Journal of Molecular Spectroscopy, 1992, 155, 430-432.	0.4	0
43	Theoretical studies of chemisorption and dimer model systems: Moeller-Plesset and configuration interaction calculations on palladium hydride (PdH), palladium carbide (PdC), palladium oxide (PdO), palladium fluoride (PdF), palladium dimer, and palladium carbonyl (PdCO). Langmuir, 1991, 7, 116-125.	1.6	34
44	Energy-adjustedab initio pseudopotentials for the second and third row transition elements: Molecular test for M2 (M=Ag, Au) and MH (M=Ru, Os). Theoretica Chimica Acta, 1991, 78, 247-266.	0.9	120
45	Energy-adjustedab initio pseudopotentials for the second and third row transition elements. Theoretica Chimica Acta, 1990, 77, 123-141.	0.9	7,627