JÃ¼rgen GrÃ¤fenstein

List of Publications by Year
in descending order

62 papers	3,625 citations	117619 34 h-index	128286 60 g-index
62 all docs	62 docs citations	62 times ranked	2846 citing authors

#	Article	IF	Citations
1	Nuclear magnetic resonance spinâ€“spin coupling constants from coupled perturbed density functional theory. Journal of Chemical Physics, 2000, 113, 3530-3547.	3.0	311
2	An Accurate Description of the Bergman Reaction Using Restricted and Unrestricted DFT:Â Stability Test, Spin Density, and On-Top Pair Densityâ€. Journal of Physical Chemistry A, 2000, 104, 1748-1761.	2.5	250
3	Can Unrestricted Density-Functional Theory Describe Open Shell Singlet Biradicals?. International Journal of Molecular Sciences, 2002, 3, 360-394.	4.1	182
4	Symmetric Halogen Bonding Is Preferred in Solution. Journal of the American Chemical Society, 2012, 134, 5706-5715.	13.7	159
5	The impact of the self-interaction error on the density functional theory description of dissociating radical cations: Ionic and covalent dissociation limits. Journal of Chemical Physics, 2004, 120, 524-539.	3.0	141
6	The combination of density functional theory with multi-configuration methods â€“ CAS-DFT. Chemical Physics Letters, 2000, 316, 569-577.	2.6	139
7	Can density functional theory describe multi-reference systems? Investigation of carbenes and organic biradicals. Physical Chemistry Chemical Physics, 2000, 2, 2091-2103.	2.8	135
8	Development of a CAS-DFT method covering non-dynamical and dynamical electron correlation in a balanced way. Molecular Physics, 2005, 103, 279-308.	1.7	109
9	Effect of the self-interaction error for three-electron bonds: On the development of new exchange-correlation functionals. Physical Chemistry Chemical Physics, 2004, 6, 1096-1112.	2.8	107
10	Density functional theory for open-shell singlet biradicals. Chemical Physics Letters, 1998, 288, 593-602.	2.6	103
11	Counterion influence on the Nâ€“Iâ€“N halogen bond. Chemical Science, 2015, 6, 3746-3756.	7.4	100
12	An efficient algorithm for the density-functional theory treatment of dispersion interactions. Journal of Chemical Physics, 2009, 130, 124105.	3.0	98
13	Calculation and analysis of NMR spinâ€“spin coupling constants. Physical Chemistry Chemical Physics, 2007, 9, 2791-2816.	2.8	95
14	On the diagnostic value of (Åœ2) in Kohn-Sham density functional theory. Molecular Physics, 2001, 99, 981-989.	1.7	89
15	Substituent Effects on the [Nâ€“Iâ€“N]⁺ Halogen Bond. Journal of the American Chemical Society, 2016, 138, 9853-9863.	13.7	89
16	Long-range and short-range Coulomb correlation effects as simulated by Hartree-Fock, local density approximation, and generalized gradient approximation exchange functionals. Theoretical Chemistry Accounts, 2003, 109, 22-35.	1.4	81
17	Symmetry of [Nâ€“Xâ€“N]⁺halogen bonds in solution. Chemical Communications, 2012, 48, 1458-1460.	4.1	76
18	Andersenâ€™s force theorem and the local stress field. Physical Review B, 1996, 53, 7143-7146.	3.2	75

#	Article	IF	Citations
19	Solvent effects on halogen bond symmetry. CrystEngComm, 2013, 15, 3087.	2.6	66
20	The nature of [Nâ€“Clâ€“N]⁺and [Nâ€“Fâ€“N]⁺halogen bonds in solution. Chemical Science, 2014, 5, 3226-3233.	7.4	66
21	Influence of the self-interaction error on the structure of the DFT exchange hole. Chemical Physics Letters, 2002, 352, 469-478.	2.6	65
22	Halogen Bonding: A Powerful Tool for Modulation of Peptide Conformation. Biochemistry, 2017, 56, 3265-3272.	2.5	65
23	Avoiding singularity problems associated with meta-GGA (generalized gradient approximation) exchange and correlation functionals containing the kinetic energy density. Journal of Chemical Physics, 2007, 127, 214103.	3.0	62
24	Quantum-mechanical stress and a generalized virial theorem for clusters and solids. Physical Review B, 1988, 37, 8167-8178.	3.2	59
25	Halogen Bond Asymmetry in Solution. Journal of the American Chemical Society, 2018, 140, 13503-13513.	13.7	57
26	What correlation effects are covered by density functional theory?. Molecular Physics, 2000, 98, 1639-1658.	1.7	55
27	Efficient density-functional theory integrations by locally augmented radial grids. Journal of Chemical Physics, 2007, 127, 164113.	3.0	53
28	Carbonâ€™s Three-Center, Four-Electron Tetrel Bond, Treated Experimentally. Journal of the American Chemical Society, 2018, 140, 17571-17579.	13.7	53
29	Analysis of the Transmission Mechanism of NMR Spinâ^'Spin Coupling Constants Using Fermi Contact Spin Density Distribution, Partial Spin Polarization, and Orbital Currents:â€‰ XHn Molecules. Journal of Physical Chemistry A, 2003, 107, 7043-7056.	2.5	51
30	The self-interaction error and the description of non-dynamic electron correlation in density functional theory. Theoretical Chemistry Accounts, 2009, 123, 171-182.	1.4	51
31	Valence-band structure of group-IV semiconductors by means of local increments. Physical Review B, 1997, 55, 13588-13597.	3.2	43
32	4-Oxo-2,3,5,6-tetrafluorocyclohexa-2,5-dienylideneâ€”A Highly Electrophilic Triplet Carbene. Chemistry - A European Journal, 2000, 6, 4567-4579.	3.3	43
33	Analysis of the NMR through-space coupling mechanism between 19F atoms. Chemical Physics Letters, 2004, 394, 5-13.	2.6	40
34	Computation of the valence band of diamond by means of local increments. Chemical Physics Letters, 1993, 215, 611-616.	2.6	37
35	Analysis of the NMR Spinâ^'Spin Coupling Mechanism Across a Hâ^'Bond:â€‰ Nature of the H-Bond in Proteins. Journal of Physical Chemistry B, 2004, 108, 1115-1129.	2.6	34
36	Î±,3-Didehydro-5-methyl-6-hydroxytoluene:Â Matrix Isolation of a Diradical Related to the Neocarzinostatin Chromophore. Journal of the American Chemical Society, 1998, 120, 8480-8485.	13.7	33

#	Article	IF	Citations
37	Analysis of the paramagnetic spinâ€“orbit transmission mechanism for NMR spinâ€“spin coupling constants using the paramagnetic spinâ€“orbit density distribution. Chemical Physics Letters, 2004, 383, 332-342.	2.6	33
38	Naphthalene Derivatives from the Roots of Pentas parvifolia and Pentas bussei. Journal of Natural Products, 2016, 79, 2181-2187.	3.0	32
39	The ozoneâ€“acetylene reaction: concerted or non-concerted reaction mechanism? A quantum chemical investigation. Chemical Physics Letters, 2001, 347, 268-276.	2.6	25
40	The¹⁵N NMR chemical shift in the characterization of weak halogen bonding in solution. Faraday Discussions, 2017, 203, 333-346.	3.2	25
41	Analysis of the spin-dipole transmission mechanism for NMR spinâ€“spin coupling constants using orbital contributions, spin polarization, and spin-dipole energy density distribution. Chemical Physics Letters, 2004, 387, 415-427.	2.6	24
42	Interplay between FÃ¶rster and Dexter Energy Transfer Rates in Isomeric Donorâ€“Bridgeâ€“Acceptor Systems. Journal of Physical Chemistry A, 2020, 124, 7219-7227.	2.5	20
43	Investigation of the Ï€ Character of a Câ^'C Bond with the Help of the Diamagnetic and Paramagnetic Spinâ^'Orbit Term of the NMR Spinâ^'Spin Coupling Constant. Journal of Physical Chemistry A, 2004, 108, 4520-4535.	2.5	18
44	Ab initioground-state correlation calculations for semiconductors with the local ansatz. Physical Review B, 1995, 51, 10556-10567.	3.2	17
45	Analysis of long-range NMR spinâ€“spin coupling in polyenes and the Ï€-mechanism. Physical Chemistry Chemical Physics, 2005, 7, 452-462.	2.8	17
46	Trimesitylsilylium cation verification of a free silylium cation in solution by NMR chemical shift calculations. Chemical Physics Letters, 1997, 279, 9-16.	2.6	16
47	Decomposition of nuclear magnetic resonance spinâ€“spin coupling constants into active and passive orbital contributions. Journal of Chemical Physics, 2004, 120, 9952-9968.	3.0	16
48	Systematic strategy for decoding the NMR spinâ€“spin coupling mechanism: the J-OC-PSP method. Magnetic Resonance in Chemistry, 2004, 42, S138-S157.	1.9	13
49	A computational study of the enantioselective addition of n-BuLi to benzaldehyde in the presence of a chiral lithium N,P amide. Organic and Biomolecular Chemistry, 2012, 10, 2807.	2.8	12
50	Aggregation and Solvation of Chiral N,Pâ€Amide Ligands in Coordinating Solvents: A Computational and NMR Spectroscopic Study. ChemPlusChem, 2012, 77, 799-806.	2.8	11
51	Local quantum mechanical stress in clusters and crystals. Physica Scripta, 1988, 37, 370-372.	2.5	10
52	Unusual long-range spin-spin coupling in fluorinated polyenes: A mechanistic analysis. Journal of Chemical Physics, 2007, 127, 174704.	3.0	10
53	One-electron versus electronâ€“electron interaction contributions to the spinâ€“spin coupling mechanism in nuclear magnetic resonance spectroscopy: Analysis of basic electronic effects. Journal of Chemical Physics, 2004, 121, 12217.	3.0	9
54	Elucidation of the Electronic Structure of Molecules with the Help of NMR Spinâ^'Spin Coupling Constants:Â The FH Molecule. Journal of Physical Chemistry A, 2005, 109, 2325-2339.	2.5	9

#	Article	IF	Citations
55	Comment on â€˜â€˜Stress field in quantum systemsâ€™â€™. Physical Review B, 1990, 41, 3245-3247.	3.2	8
56	Efficient calculation of NMR isotopic shifts: Difference-dedicated vibrational perturbation theory. Journal of Chemical Physics, 2019, 151, 244120.	3.0	7
57	Sum rule for planar jellium surfaces treated within the Kohn-Sham local-density approximation. Physical Review B, 1992, 46, 1715-1718.	3.2	6
58	Calculated Fermi Surface Characteristics of the Noble Metals. Physica Status Solidi (B): Basic Research, 1988, 147, 575-582.	1.5	4
59	Anisotropic electron-impurity scattering rates of dilute noble-metal alloys: a comparison with surface state resonance data. Journal of Physics F: Metal Physics, 1988, 18, 731-743.	1.6	4
60	Photochemically Induced Aryl Azide Rearrangement: Solution NMR Spectroscopic Identification of the Rearrangement Product. Journal of Organic Chemistry, 2017, 82, 1812-1816.	3.2	3
61	The Structure of the â€œVibration Holeâ€•around an Isotopic Substitutionâ€”Implications for the Calculation of Nuclear Magnetic Resonance (NMR) Isotopic Shifts. Molecules, 2020, 25, 2915.	3.8	3
62	An Alternative Approach to Calculate the Hydrostatic Pressure in Solids. Physica Status Solidi (B): Basic Research, 1990, 158, K133.	1.5	1