Magdalena Pecul-Kudelska

List of Publications by Year
in descending order

83	2,983	117453	182168
papers	citations	34 h-index	51 g-index

89	89	89	2214
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Nuclear magnetic resonance parameters in Zn2, Cd2 and Hg2 dimers: relativistic calculations. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	4
2	Relativistic Four-Component DFT Calculations of Vibrational Frequencies. Journal of Physical Chemistry A, 2021, 125, 10315-10320.	1.1	2
3	Nuclear Magnetic Resonance parameters of mercury atom and water molecule complex: Relativistic calculations. Chemical Physics Letters, 2019, 736, 136775.	1.2	4
4	Spinâ€“spin coupling constants in $$hbox {HC}{equiv }hbox {CXH}_3$$ HC â‰¡ CXH 3 molecules; $$hbox {X}{=}. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	7
5	Thioflavinâ€…T: Electronic Circular Dichroism and Circularly Polarized Luminescence Induced by Amyloid Fibrils. ChemPhysChem, 2016, 17, 2931-2937.	1.0	33
6	The Relativistic Effects on the Carbonâ€“Carbon Coupling Constants Mediated by a Heavy Atom. Journal of Physical Chemistry A, 2016, 120, 5624-5634.	1.1	10
7	Electronic Circular Dichroism of Fluorescent Proteins: A Computational Study. Journal of Physical Chemistry B, 2015, 119, 3377-3386.	1.2	13
8	A computational protocol for the study of circularly polarized phosphorescence and circular dichroism in spin-forbidden absorption. Physical Chemistry Chemical Physics, 2015, 17, 19079-19086.	1.3	15
9	Induced circular dichroism of thioflavin T interacting with acetylcholinesterase: A computational study. Chemical Physics, 2015, 463, 82-87.	0.9	1
10	The selectivity of diglycolamide (TODGA) and bis-triazine-bipyridine (BTBP) ligands in actinide/lanthanide complexation and solvent extraction separation â€“ a theoretical approach. Dalton Transactions, 2015, 44, 2657-2666.	1.6	91
11	The influence of a presence of a heavy atom on the spin-spin coupling constants between two light nuclei in organometallic compounds and halogen derivatives. Journal of Chemical Physics, 2014, 140, 024319.	1.2	8
12	What Factors Influence the Metalâ€“Proton Spinâ€“Spin Coupling Constants in Mercury- and Cadmium-Substutited Rubredoxin?. Journal of Physical Chemistry A, 2014, 118, 4471-4479.	1.1	10
13	Electronic Circular Dichroism Spectroscopy in Structural Analysis of Biomolecular Systems. Challenges and Advances in Computational Chemistry and Physics, 2014, , 161-177.	0.6	1
14	The Influence of a Presence of a Heavy Atom on ¹³C Shielding Constants in Organomercury Compounds and Halogen Derivatives. Journal of Chemical Theory and Computation, 2013, 9, 1909-1917.	2.3	24
15	Circular Dichroism and Optical Rotation of Lactamide and 2-Aminopropanol in Aqueous Solution. Journal of Physical Chemistry B, 2013, 117, 5136-5147.	1.2	16
16	A comparison of two-component and four-component approaches for calculations of spin-spin coupling constants and NMR shielding constants of transition metal cyanides. Journal of Chemical Physics, 2012, 137, 014311.	1.2	34
17	Vibrational Optical Activity of Cysteine in Aqueous Solution: A Comparison of Theoretical and Experimental Spectra. Journal of Physical Chemistry B, 2012, 116, 4976-4990.	1.2	42
18	Linear and nonlinear second order susceptibilities of molecular crystals. , 2012, , .		0

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19	A simple scheme for magnetic balance in four-component relativistic Kohnâ€“Sham calculations of nuclear magnetic resonance shielding constants in a Gaussian basis. Journal of Chemical Physics, 2012, 136, 014108.	1.2	80
20	Spinâ€“Spin Artificial DNA Intercalated with Silver Cations: Theoretical Prediction. ChemPhysChem, 2012, 13, 1332-1338.	1.0	8
21	The optical activity of Î²,Î³-enones in ground and excited states using circular dichroism and circularly polarized luminescence. Physical Chemistry Chemical Physics, 2011, 13, 643-650.	1.3	45
22	Theoretical Prediction of the Spinâ€“Spin Coupling Constants between an Axis and Macrocycle of a Rotaxane. Journal of Physical Chemistry A, 2011, 115, 10795-10800.	1.1	6
23	Explicit versus Implicit Solvent Modeling of Raman Optical Activity Spectra. Journal of Physical Chemistry B, 2011, 115, 4128-4137.	1.2	92
24	DFT calculations of ³¹P spinâ€“spin coupling constants and chemical shift in dioxaphosphorinanes. Magnetic Resonance in Chemistry, 2011, 49, 399-404.	1.1	19
25	The aqueous Raman optical activity spectra of 4(R)â€hydroxyproline: theory and experiment. Journal of Raman Spectroscopy, 2010, 41, 1200-1210.	1.2	16
26	Circularly polarized component in surface-enhanced Raman spectra. Chemical Physics Letters, 2010, 496, 86-90.	1.2	35
27	New applications and challenges for computational ROA spectroscopy. Chirality, 2009, 21, E98-104.	1.3	39
28	Spinâ€“Spin Coupling Constants Transmitted through Ir¿Hâ‹…â‹…â‹…Hï£¿N Dihydrogen Bonds. ChemPhysChem, 2009, 10, 1247-1259.	1.0	15
29	The quantum-chemical calculation of NMR indirect spinâ€“spin coupling constants. Progress in Nuclear Magnetic Resonance Spectroscopy, 2008, 53, 249-268.	3.9	252
30	A Chiral â€œFrozenâ€•Hydrogen Bonding in C₄â€Symmetric Inherently Chiral Resorcin[4]arenes: NMR, Xâ€ray, Circular Dichroism, and Theoretical Study. European Journal of Organic Chemistry, 2008, 2008, 3069-3078.	1.2	28
31	Theoretical investigation on the linear and nonlinear susceptibilities of urea crystal. Journal of Chemical Physics, 2008, 128, 244713.	1.2	26
32	Electronic circular dichroism of disulphide bridge: Ab initio quantum-chemical calculations. Journal of Chemical Physics, 2007, 127, 085102.	1.2	18
33	Solvent Effects on Raman Optical Activity Spectra Calculated Using the Polarizable Continuum Model. Journal of Physical Chemistry A, 2006, 110, 2807-2815.	1.1	59
34	On the calculations of the nuclear spinâ€“spin coupling constants in small water clusters. Chemical Physics, 2006, 326, 431-444.	0.9	18
35	Conformational structures and optical rotation of serine and cysteine. Chemical Physics Letters, 2006, 418, 1-10.	1.2	68
36	Theoretical simulation of the ROA spectra of neutral cysteine and serine. Chemical Physics Letters, 2006, 427, 166-176.	1.2	21

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37	Relativistic calculation of NMR properties of XeF2, XeF4 and XeF6. Chemical Physics Letters, 2006, 427, 281-288.	1.2	37
38	High-order correlation effects on dynamic hyperpolarizabilities and their geometric derivatives: A comparison with density functional results. Journal of Chemical Physics, 2006, 124, 114101.	1.2	46
39	Density functional and coupled cluster calculations of dynamic hyperpolarizabilities and their geometry derivatives. Chemical Physics Letters, 2005, 404, 217-226.	1.2	36
40	A protein backbone Ï^ and Ït angle dependence of 2J N (i) ,CÎ±1;(i - 1): The new NMR experiment and quantum chemical calculations. Journal of Biomolecular NMR, 2005, 31, 87-95.	1.6	10
41	Ab initio calculation of vibrational Raman optical activity. International Journal of Quantum Chemistry, 2005, 104, 816-829.	1.0	67
42	The Ab Initio Calculation of Optical Rotation and Electronic Circular Dichroism. Advances in Quantum Chemistry, 2005, 50, 185-212.	0.4	109
43	Theoretical Studies of Nuclear Magnetic Resonance Parameters for the Proton-Exchange Pathways in Porphyrin and Porphycene. Journal of Physical Chemistry A, 2005, 109, 4162-4171.	1.1	22
44	Chiral bias of amyloid fibrils revealed by the twisted conformation of Thioflavin T: An induced circular dichroism/DFT study. FEBS Letters, 2005, 579, 6601-6603.	1.3	83
45	Polarizable continuum model study of solvent effects on electronic circular dichroism parameters. Journal of Chemical Physics, 2005, 122, 024106.	1.2	58
46	Improper Hydrogen Cï£¿Hâ‹…â‹…â‹…O Bonds Cause Self-Association ofÎ±,Î²-Enaminoketones Containing Fluorosubstituted Alkyl Groups. ChemPhysChem, 2004, 5, 209-215.	1.0	18
47	Solvent effects on the spinâ€“spin coupling constants of acetylene revisited: supermolecular and polarizable continuum model calculations. Magnetic Resonance in Chemistry, 2004, 42, S128-S137.	1.1	26
48	The nature of the rotational barriers in simple carbonyl compounds. Tetrahedron, 2004, 60, 179-185.	1.0	8
49	Density functional theory calculation of electronic circular dichroism using London orbitals. Chemical Physics Letters, 2004, 388, 110-119.	1.2	123
50	Electric field effects on the shielding constants of noble gases: A four-component relativistic Hartree-Fock study. Journal of Chemical Physics, 2004, 121, 3051-3057.	1.2	40
51	Conformational Effects on the Optical Rotation of Alanine and Proline. Journal of Physical Chemistry A, 2004, 108, 4269-4276.	1.1	103
52	Potential Energy and Spinâ^'Spin Coupling Constants Surface of Glycolaldehyde. Journal of Physical Chemistry A, 2004, 108, 2758-2769.	1.1	18
53	Spin-Spin Coupling Constants with HF and DFT Methods. , 2004, , 101-121.		25
54	Full configuration-interaction and coupled-cluster calculations of the indirect spinâ€“spin coupling constant of BH. Chemical Physics Letters, 2003, 368, 172-176.	1.2	32

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55	Relativistic effects on the electric polarizabilities and their geometric derivatives for hydrogen halides and dihalogens â€“ a Diracâ€“Hartreeâ€“Fock study. Chemical Physics Letters, 2003, 370, 578-588.	1.2	17
56	Calculations of hydrogen-bond-transmitted indirect nuclear spinâ€“spin couplings: a comparison of density-functional and ab initio methods. Chemical Physics Letters, 2003, 372, 476-484.	1.2	27
57	Characterization of dihydrogen-bonded Dâ€“Hâ‹¯Hâ€“A complexes on the basis of infrared and magnetic resonance spectroscopic parameters. Journal of Chemical Physics, 2003, 119, 5094-5104.	1.2	66
58	Raman optical activity spectra: basis set and electron correlation effects. Molecular Physics, 2003, 101, 2073-2081.	0.8	36
59	The Spinâ€“Spin Coupling Constants in Ethane, Methanol and Methylamine: A Comparison of DFT, MCSCF and CCSD Results. International Journal of Molecular Sciences, 2003, 4, 143-157.	1.8	39
60	Ab Initio Calculations of the Intermolecular Nuclear Spin-Spin Coupling Constants. Computational Chemistry - Reviews of Current Trends, 2003, , 131-160.	0.4	4
61	A full configuration interaction calculation of the density dependence of the3He shielding constant. Molecular Physics, 2002, 100, 447-451.	0.8	9
62	Ab initiostudy of magnetochiral birefringence. Journal of Chemical Physics, 2002, 117, 6417-6428.	1.2	51
63	Linear response coupled cluster calculation of Raman scattering cross sections. Journal of Chemical Physics, 2002, 116, 1259-1268.	1.2	28
64	Vibrational Raman and Raman Optical Activity Spectra ofd-Lactic Acid,d-Lactate, andd-Glyceraldehyde:Â Ab Initio Calculations. Journal of Physical Chemistry A, 2002, 106, 11008-11016.	1.1	94
65	Interaction of 2-mercaptoethanesulfonate monolayers on silver with sodium cations. Journal of Raman Spectroscopy, 2002, 33, 796-800.	1.2	27
66	The effect of triple excitations in coupled cluster calculations of Raman scattering cross-sections. Chemical Physics Letters, 2002, 355, 327-338.	1.2	21
67	The spinâ€“spin coupling constants in the ammonia dimer. Chemical Physics Letters, 2002, 360, 272-282.	1.2	15
68	The 19Fâ€“1H coupling constants transmitted through covalent, hydrogen bond, and van der Waals interactions. Journal of Chemical Physics, 2001, 115, 5498-5506.	1.2	43
69	Ab initio calculations of the NMR spectra of [1.1.1]propellane and bicyclo[1.1.1]pentane. Physical Chemistry Chemical Physics, 2001, 3, 1986-1991.	1.3	36
70	Benchmark calculations of the shielding constants in the water dimer. Chemical Physics Letters, 2001, 333, 139-145.	1.2	23
71	The nuclear spinâ€“spin coupling constants in methanol and methylamine: geometry and solvent effects. Chemical Physics, 2000, 255, 137-148.	0.9	15
72	Singlet excited states of Be2. Journal of Chemical Physics, 2000, 112, 3671-3679.	1.2	34

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73	Comprehensive ab initio studies of nuclear magnetic resonance shielding and coupling constants in XHâ‹¯O hydrogen-bonded complexes of simple organic molecules. Journal of Chemical Physics, 2000, 112, 7930-7938.	1.2	49
74	Singlet excitations and dipole polarizabilities of Li2, Li4 and Li8 clusters. Molecular Physics, 2000, 98, 1455-1465.	0.8	11
75	The nuclear spinâ€“spin coupling constant in He2. Journal of Chemical Physics, 2000, 113, 10835-10836.	1.2	31
76	Nuclear Magnetic Shielding and Spinâ^'Spin Coupling of 1,2-13C-Enriched Acetylene in Gaseous Mixtures with Xenon and Carbon Dioxide. Journal of Physical Chemistry A, 2000, 104, 5955-5958.	1.1	70
77	The Shielding Constants and Scalar Couplings in Nâ^'HÂ·Â·Â·OC and Nâ^'HÂ·Â·Â·NC Hydrogen Bonded Systems:Â An ab Initio MO Study. Journal of Physical Chemistry A, 2000, 104, 8105-8113.	1.1	59
78	The influence of electrostatic and dispersion interactions on the NMR parameters of acetylene. Chemical Physics, 1999, 248, 27-40.	0.9	13
79	The geometry dependence of the spinâ€“spin coupling constants in ethane: a theoretical study. Chemical Physics Letters, 1999, 305, 139-146.	1.2	25
80	The nuclear spinâ€“spin coupling constants in the water dimer. Chemical Physics Letters, 1999, 308, 486-494.	1.2	37
81	Solvent effects on NMR spectrum of acetylene calculated by ab initio methods. Chemical Physics, 1998, 234, 111-119.	0.9	49
82	Ab initio calculation of and NMR shielding constants in solid acetylene. Solid State Nuclear Magnetic Resonance, 1997, 8, 139-145.	1.5	16
83	Properties and Spectroscopies. , 0, , 125-312.		3