Grzegorz ChaÅ‚asÃ-nski

List of Publications by Year
in descending order

79 papers	3,416 citations	218677 26 h-index	144013 57 g-index
79 all docs	79 docs citations	79 times ranked	1908 citing authors

#	Article	IF	Citations
1	Reassessing the Role of Ïƒ Holes in Noncovalent Interactions: It is Pauli Repulsion that Counts. Frontiers in Chemistry, 2022, 10, 858946.	3.6	5
2	Assessment of SAPT(DFT) with meta-GGA functionals. Journal of Molecular Modeling, 2020, 26, 102.	1.8	7
3	Toward Heterolytic Bond Dissociation of Dihydrogen: The Study of Hydrogen in Arsenolite under High Pressure. Journal of Physical Chemistry C, 2019, 123, 16868-16872.	3.1	6
4	Assessment of Newest Meta-GGA Hybrids for Late Transition Metal Reactivity: Fractional Charge and Fractional Spin Perspective. Journal of Physical Chemistry C, 2019, 123, 8047-8056.	3.1	17
5	How and Why Does Helium Permeate Nonporous Arsenolite Under High Pressure?. ChemPhysChem, 2018, 19, 857-864.	2.1	10
6	The nature of three-body interactions in DFT: Exchange and polarization effects. Journal of Chemical Physics, 2017, 147, 084106.	3.0	15
7	Theoretical study of the buffer-gas cooling and trapping of CrH(X6Î£+) by 3He atoms. Journal of Chemical Physics, 2016, 145, 214305.	3.0	4
8	Employing Range Separation on the meta-GGA Rung: New Functional Suitable for Both Covalent and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2016, 12, 3662-3673.	5.3	10
9	Noncovalent interactions determine the conformation of aurophilic complexes with 2-mercapto-4-methyl-5-thiazoleacetic acid ligands. Dalton Transactions, 2015, 44, 13641-13650.	3.3	5
10	Tuned range-separated hybrid functionals in the symmetry-adapted perturbation theory. Journal of Chemical Physics, 2014, 141, 134120.	3.0	18
11	Density functional theory approach to gold-ligand interactions: Separating true effects from artifacts. Journal of Chemical Physics, 2014, 140, 244313.	3.0	14
12	Range-Separated meta-GGA Functional Designed for Noncovalent Interactions. Journal of Chemical Theory and Computation, 2014, 10, 4297-4306.	5.3	17
13	Theoretical Studies of Potential Energy Surface and Bound States of the Strongly Bound He(¹S)â€“BeO (¹Î£⁺) Complex. Journal of Physical Chemistry A, 2013, 117, 6657-6663.	2.5	15
14	Density-Dependent Onset of the Long-Range Exchange: A Key to Donorâ€“Acceptor Properties. Journal of Physical Chemistry A, 2013, 117, 11580-11586.	2.5	26
15	First-principle interaction potentials for metastable He(3S) and Ne(3P) with closed-shell molecules: Application to Penning-ionizing systems. Journal of Chemical Physics, 2013, 139, 014307.	3.0	18
16	Dispersion-free component of non-covalent interaction via mutual polarization of fragment densities. Journal of Chemical Physics, 2012, 136, 204109.	3.0	8
17	Interactions of ThO(X) with He, Ne and Ar from the ab initio coupled cluster and symmetry adapted perturbation theory calculations. Chemical Physics, 2012, 399, 50-58.	1.9	5
18	Aurophilic Interactions from Wave Function, Symmetry-Adapted Perturbation Theory, and Rangehybrid Approaches. Journal of Chemical Theory and Computation, 2011, 7, 2399-2407.	5.3	37

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19	Derivation of the supermolecular interaction energy from the monomer densities in the density functional theory. Chemical Physics Letters, 2010, 486, 160-165.	2.6	20
20	Density Functional Theory Approach to Noncovalent Interactions via Monomer Polarization and Pauli Blockade. Physical Review Letters, 2010, 104, 163001.	7.8	34
21	A density functional theory approach to noncovalent interactions via interacting monomer densities. Physical Chemistry Chemical Physics, 2010, 12, 14686.	2.8	9
22	Study of KrO^{â˜’} and KrO via Slow Photoelectron Velocity-Map Imaging Spectroscopy and ab Initio Calculations. Journal of Physical Chemistry A, 2009, 113, 14439-14446.	2.5	9
23	The nature of interactions between clusters of Mg and Zn with HCN from symmetry-adapted perturbation theory based of DFT. Journal of Chemical Physics, 2009, 130, 224704.	3.0	5
24	Interactions of transition metal atoms in high-spin states: Cr2, Scâ€“Cr, and Scâ€“Kr. Journal of Chemical Physics, 2007, 127, 244302.	3.0	13
25	Diffuse basis functions for small-core relativistic pseudopotential basis sets and static dipole polarizabilities of selected lanthanides La, Sm, Eu, Tm and Yb. Structural Chemistry, 2007, 18, 769-772.	2.0	33
26	Interaction potentials for Brâ˜’â€“Rg (Rg=Heâ€“Rn): Spectroscopy and transport coefficients. Journal of Chemical Physics, 2006, 125, 064305.	3.0	16
27	van der Waals interactions and dipole polarizabilities of lanthanides: Tm(F2)â€“He and Yb(S1)â€“He potentials. Journal of Chemical Physics, 2006, 124, 114301.	3.0	23
28	Interactions in Open-Shell Clusters:Â Ab Initio Study of Pre-reactive Complex O(3P) + HClâ€. Journal of Physical Chemistry A, 2005, 109, 11484-11494.	2.5	7
29	Conformational analysis of N-benzyl-N-o-tolyl-p-methylbenzene-sulfonamides from dynamic 1H NMR experiments and theoretical calculations. Computational and Theoretical Chemistry, 2004, 680, 5-13.	1.5	3
30	Characterization of Ar[sub n]O[sup â˜’] clusters from ab initio and diffusion Monte Carlo calculations. Journal of Chemical Physics, 2003, 118, 2748.	3.0	8
31	Modeling of the three-body effects in the Ar[sub 2]O[sup â˜’] trimer from ab initio calculations. Journal of Chemical Physics, 2003, 118, 2731.	3.0	6
32	Modeling of the Three-Body Effects in the Neutral Trimers in the Quartet State by ab initio Calculations. H3, Na3, and Na2B. Collection of Czechoslovak Chemical Communications, 2003, 68, 587-626.	1.0	3
33	Modeling of adiabatic and diabatic potential energy surfaces of Cl(2P)â‹¯H2(1â˜‘g+) prereactive complex from ab initio calculations. Journal of Chemical Physics, 2002, 117, 4709-4719.	3.0	17
34	Ab initio simulations of the KrOâ˜’ anion photoelectron spectra. Journal of Chemical Physics, 2002, 117, 2629-2634.	3.0	16
35	Ab Initio Calculations and Modeling of Three-Dimensional Adiabatic and Diabatic Potential Energy Surfaces of Br(2P)Â·Â·Â·H2(1Î£+) Pre-Reactive Complex. Journal of Physical Chemistry A, 2002, 106, 7362-7368.	2.5	7
36	Ab initio calculations and modeling of three-body forces in Ar2H2O. International Journal of Quantum Chemistry, 2002, 90, 1215-1231.	2.0	0

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37	Ab initio calculations and modeling of three-dimensional adiabatic and diabatic potential energy surfaces of F(2P)Â·Â·Â·H2(1Î£+) Van der Waals complex. International Journal of Quantum Chemistry, 2002, 90, 1038-1048.	2.0	11
38	Collision and transport properties of Rg+Cl(2P) and Rg+Clâ¯(1S) (Rg=Ar,â€ŠKr) fromab initiopotentials. Journal of Chemical Physics, 2001, 114, 9919-9928.	3.0	36
39	Ab initiocalculations of adiabatic and diabatic potential energy surfaces of Cl(2P)â‹¯HCl(1Î£+) van der Waals complex. Journal of Chemical Physics, 2001, 115, 3085-3098.	3.0	41
40	Ab initiozero electron kinetic energy spectroscopy of the ArClâ¯ and KrClâ¯ anions. Journal of Chemical Physics, 2001, 114, 9929-9937.	3.0	20
41	Ab initio potential energy surface for the Ar(1S)+OH(X2Î) interaction and bound rovibrational states. Journal of Chemical Physics, 2000, 112, 4952-4958.	3.0	48
42	State of the Art and Challenges of the ab Initio Theory of Intermolecular Interactions. Chemical Reviews, 2000, 100, 4227-4252.	47.7	478
43	Ab initio based study of the ArOâ¯ photoelectron spectra: Selectivity of spinâ€“orbit transitions. Journal of Chemical Physics, 2000, 112, 5852-5865.	3.0	31
44	Structure and energetics of ArnNOâ¯ clusters from ab initio calculations. Journal of Chemical Physics, 2000, 112, 10895-10904.	3.0	7
45	A three-dimensional potential energy surface for He+Cl2 (Bâ€Š3Î0u+): Ab initio calculations and a multiproperty fit. Journal of Chemical Physics, 1999, 111, 997-1007.	3.0	44
46	An ab initio study of the Arâ€“HCN complex. Journal of Chemical Physics, 1999, 110, 1416-1423.	3.0	21
47	Many-body exchange effects in clusters of rare gases with a chromophore: He2CO2. Chemical Physics, 1998, 239, 573-591.	1.9	6
48	Ab initio study of energy, structure and dynamics of the waterâ€“carbon dioxide complex. Journal of Chemical Physics, 1998, 109, 3919-3927.	3.0	51
49	From Intermolecular Interactions to Incipient Chemical Bond. Collection of Czechoslovak Chemical Communications, 1998, 63, 1473-1484.	1.0	11
50	Ab initiostudy of the O2(Xâ€‰3Î£gâ¯)+Ar(1S) van der Waals interaction. Journal of Chemical Physics, 1997, 106, 7731-7737.	3.0	24
51	Arî—¸C2H2: a challenging system for ab initio calculations. Journal of Molecular Structure, 1997, 436-437, 387-400.	3.6	14
52	Comment on â€œA possible definition of basis set superposition errorâ€• Chemical Physics Letters, 1995, 241, 140-145.	2.6	23
53	Site-site function and successive reaction counterpoise calculation of basis set superposition error for proton transfer. Computational and Theoretical Chemistry, 1995, 342, 153-159.	1.5	6
54	On the nature of the interaction energy in the Ar-Cl2 complex. Computational and Theoretical Chemistry, 1994, 307, 187-199.	1.5	26

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55	Origins of Structure and Energetics of van der Waals Clusters from ab Initio Calculations. Chemical Reviews, 1994, 94, 1723-1765.	47.7	781
56	Perturbation analysis of the supermolecule interaction energy and the basis set superposition error. Chemical Physics Letters, 1992, 197, 591-598.	2.6	40
57	Basis set superposition error in proton transfer potentials. Chemical Physics Letters, 1992, 196, 384-389.	2.6	27
58	Ab initio studies of the structure and energies of the nitric oxide-helium and nitric oxide-argon complexes. The Journal of Physical Chemistry, 1990, 94, 3450-3454.	2.9	9
59	Anisotropy of correlation effects in hydrogen-bonded systems: the HF dimer. Chemical Physics Letters, 1989, 161, 532-538.	2.6	6
60	The Ab initio energy and structure of hydride-hydrogen (H-(H2)2). The Journal of Physical Chemistry, 1989, 93, 621-625.	2.9	18
61	Van der Waals minima in excited states by MÃ¸ller-Plesset perturbation theory: The a 3Î£u+ State of He2 And the 3Ï€ state of MgHe. Chemical Physics Letters, 1988, 148, 289-295.	2.6	19
62	Weak interactions between small systems. Models for studying the nature of intermolecular forces and challenging problems for ab initio calculations. Chemical Reviews, 1988, 88, 943-962.	47.7	266
63	Propensity rules for vibration-rotation-induced electron detachment of diatomic anions: application to amidogen(1-) ion .fwdarw. imidogen + electron. The Journal of Physical Chemistry, 1988, 92, 3086-3091.	2.9	19
64	Proper correction for the basis set superposition error in SCF calculations of intermolecular interactions. Molecular Physics, 1987, 61, 233-247.	1.7	138
65	Ab initio studies of the structure and energetics of the hydride (hydrogen) complex. The Journal of Physical Chemistry, 1987, 91, 6151-6158.	2.9	19
66	The impact of higher polarization functions of second-order dispersion energy. Partial wave expansion and damping phenomenon for He2. Chemical Physics, 1987, 111, 271-283.	1.9	93
67	Intramolecular correlation correction to the first-order interaction energy between H2 molecules and its influence on the H2-H2 potential surface. Molecular Physics, 1986, 57, 427-439.	1.7	22
68	Dimer centred basis set in the calculations of the first-order interaction energy with CI wavefunction. Molecular Physics, 1985, 54, 1173-1184.	1.7	39
69	Effective basis sets for calculations of exchange-repulsion energy. International Journal of Quantum Chemistry, 1984, 26, 971-982.	2.0	69
70	Exchange-perturbation calculations of the interaction energy between Be atoms including intra-atomic correlation effects. Chemical Physics, 1983, 82, 207-213.	1.9	16
71	Perturbation calculations of the interaction energy between closed-shell Hartree-Fock atoms. Molecular Physics, 1983, 49, 1353-1373.	1.7	31
72	Ab initiocalculations of exchange repulsion between two Ar atoms. Molecular Physics, 1982, 45, 1271-1278.	1.7	13

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73	Many-orbital cluster expansion for the exchange-repulsion nonadditivity in the interaction of rare gas atoms. The neon trimer. Theoretica Chimica Acta, 1980, 56, 199-210.	0.8	38
74	Many-orbital cluster expansion for the exchange-repulsion energy in the interaction of closed-shell systems. Theoretica Chimica Acta, 1979, 52, 93-101.	0.8	26
75	Symmetry forcing and convergence properties of perturbation expansions for molecular interaction energies. International Journal of Quantum Chemistry, 1978, 14, 271-287.	2.0	128
76	On the convergence properties of the Rayleigh-SchrÃ¶dinger and the Hirschfelder-Silbey perturbation expansions for molecular interaction energies. International Journal of Quantum Chemistry, 1977, 11, 247-257.	2.0	66
77	On basis set effects in SCF calculations of the interaction energy between closed-shell atoms. Theoretica Chimica Acta, 1977, 44, 399-404.	0.8	43
78	Exchange polarization effects in the interaction of closed-shell systems. Theoretica Chimica Acta, 1977, 46, 277-290.	0.8	81
79	An exact treatment of the induction interaction between the atoms in the hydrogen molecule. Molecular Physics, 1974, 27, 649-655.	1.7	45