Malgorzata M Szczesniak

List of Publications by Citations

134 papers	5,161 citations	37 h-index	67 g-index
136 ext. papers	5,297 ext. citations	4.6 avg, IF	5.27 L-index

#	Paper	IF	Citations
134	Origins of Structure and Energetics of van der Waals Clusters from ab Initio Calculations. *Chemical Reviews*, **1994**, 94, 1723-1765	68.1	736
133	State of the Art and Challenges of the ab Initio Theory of Intermolecular Interactions. *Chemical Reviews*, **2000**, 100, 4227-4252	68.1	451
132	On the connection between the supermolecular Møller-Plesset treatment of the interaction energy and the perturbation theory of intermolecular forces. *Molecular Physics*, **1988**, 63, 205-224	1.7	291
131	Ab initio study of intermolecular potential of H2O trimer. *Journal of Chemical Physics*, **1991**, 94, 2873-2883	3.9	138
130	Correction of the basis set superposition error in SCF and MP2 interaction energies. The water dimer. *Journal of Chemical Physics*, **1986**, 84, 6328-6335	3.9	124
129	Nonadditive effects in HF and HCl trimers. *Journal of Chemical Physics*, **1989**, 91, 7048-7056	3.9	113
128	Calculations of nonadditive effects by means of supermolecular Mo/llerPlesset perturbation theory approach: Ar3 and Ar4. *Journal of Chemical Physics*, **1990**, 92, 2481-2487	3.9	97
127	Ab initio study of the potential energy surface of CH4-H2O. *Journal of Chemical Physics*, **1993**, 98, 3078-3089	3.9	95
126	Interactions between aromatic systems: dimers of benzene and s-tetrazine. *The Journal of Physical Chemistry*, **1984**, 88, 1726-1730		83
125	Intermolecular potential of the methane dimer and trimer. *Journal of Chemical Physics*, **1990**, 93, 4243-4253	3.9	81
124	Theoretical study of H2OHF and H2OHCl: Comparison with experiment. *Journal of Chemical Physics*, **1984**, 81, 5024-5030	3.9	79
123	On the role of bond functions in interaction energy calculations: Ar???HCl, Ar???H2O, (HF)2. *Journal of Chemical Physics*, **1995**, 103, 1498-1507	3.9	78
122	Ab initio study of the intermolecular potential of ArH2O. *Journal of Chemical Physics*, **1991**, 94, 2807-2816	3.9	78
121	Analysis of the potential energy surface of ArNH3. *Journal of Chemical Physics*, **1989**, 91, 7809-7817	3.9	74
120	Ab initio study of van der Waals interaction of CO2 with Ar. *Journal of Chemical Physics*, **1996**, 104, 6569-6576	3.9	67
119	The complex of N2 with H2O, D2O, and HDO: A combined ab initio and diffusion Monte Carlo study. *Journal of Chemical Physics*, **1994**, 101, 1378-1391	3.9	60
118	Mo/llerPlesset treatment of electron correlation effects in (HOHOH)*Journal of Chemical Physics*, **1982**, 77, 4586-4593	3.9	58

117	Ab initio study of intermolecular potential for ArHCl. *Journal of Chemical Physics*, **1991**, 94, 6677-6685	3.9	57
116	Ab initio study of proton transfers including effects of electron correlation. *International Journal of Quantum Chemistry*, **1983**, 23, 739-751	2.1	56
115	Supermolecular approach to many-body dispersion interactions in weak van der Waals complexes: He, Ne, and Ar trimers. *Journal of Chemical Physics*, **1994**, 101, 8860-8869	3.9	54
114	Optical absorption spectra of gold clusters Au(n) (n = 4, 6, 8,12, 20) from long-range corrected functionals with optimal tuning. *Journal of Chemical Physics*, **2012**, 137, 114302	3.9	52
113	Suppression of angular forces in collisions of non-S-state transition metal atoms. *Physical Review Letters*, **2005**, 94, 013202	7.4	51
112	Effects of external ions on the energetics of proton transfers across hydrogen bonds. *The Journal of Physical Chemistry*, **1985**, 89, 262-266		49
111	Counterpoise-corrected geometries and harmonic frequencies of N-body clusters: Application to (HF)n (n=3,4). *Journal of Chemical Physics*, **2003**, 118, 537-549	3.9	46
110	Ab initio potential energy surface for the Ar(1S)+OH(X2Π)interaction and bound rovibrational states. *Journal of Chemical Physics*, **2000**, 112, 4952-4958	3.9	46
109	Partitioning of interaction energy in van der Waals complexes involving excited state species: The He(1S)+Cl2(B 3Π) interaction. *Journal of Chemical Physics*, **1995**, 103, 10116-10127	3.9	46
108	The nonadditive interactions in the Ar2HF and Ar2HCl clusters: An ab initio study. *Journal of Chemical Physics*, **1993**, 99, 6732-6741	3.9	46
107	Ab initio study of structure and cooperativity in ammonia-hydrogen fluoride-hydrogen fluoride and phosphine-hydrogen fluoride-hydrogen fluoride. *The Journal of Physical Chemistry*, **1986**, 90, 4253-4258		46
106	Potential energy surface for dispersion interaction in water dimer and hydrogen fluoride dimer. *The Journal of Physical Chemistry*, **1990**, 94, 1781-1788		44
105	Ab initio potential energy and dipole moment surfaces, infrared spectra, and vibrational predissociation dynamics of the 35Cl⁻H2/D2 complexes. *Journal of Chemical Physics*, **2003**, 119, 12931-12945	3.9	43
104	Ab initio calculations of adiabatic and diabatic potential energy surfaces of Cl(2P)?HCl(1Σ) van der Waals complex. *Journal of Chemical Physics*, **2001**, 115, 3085-3098	3.9	41
103	A three-dimensional potential energy surface for He+Cl2 (B 3Πu+): Ab initio calculations and a multiproperty fit. *Journal of Chemical Physics*, **1999**, 111, 997-1007	3.9	41
102	Vibrational frequencies and intensities of H-bonded and Li-bonded complexes. H3N??HCl and H3N??LiCl. *Journal of Chemical Physics*, **1988**, 89, 3131-3138	3.9	39
101	Symmetry-adapted perturbation theory based on unrestricted Kohn-Sham orbitals for high-spin open-shell van der Waals complexes. *Journal of Chemical Physics*, **2012**, 137, 164104	3.9	38
100	Ab initio calculations of the interaction of He with the B 3Πu+ state of Cl2 as a function of the Cl2 internuclear separation. *Journal of Chemical Physics*, **1997**, 106, 2685-2694	3.9	37

99	Ab initio study of the van der Waals interaction of NH(X 3Σ−)with Ar(1S). *Journal of Chemical Physics*, **1998**, 108, 3235-3242	3.9	37
98	Analysis of the intermolecular potential of Ar–CH4: An ab initio study. *Journal of Chemical Physics*, **1992**, 96, 463-469	3.9	37
97	RG+Cl(2P) (RG=He, Ne, Ar) interactions: Ab initio potentials and collision properties. *Journal of Chemical Physics*, **1998**, 109, 2144-2154	3.9	36
96	Intermolecular potential of H2O???H2 in the van der Waals region. An ab initio study. *Journal of Chemical Physics*, **1992**, 96, 6039-6047	3.9	36
95	Interaction potentials of the RG-I anions, neutrals, and cations (RG = He, Ne, Ar). *Journal of Chemical Physics*, **2005**, 122, 194311	3.9	35
94	Paradigm pre-reactive van der Waals complexes: XH–X and XH–2 (X = F, Cl, Br). *International Reviews in Physical Chemistry*, **2004**, 23, 541-571	7	35
93	Collision and transport properties of Rg+Cl(2P) and Rg+Cl–(1S) (Rg=Ar, Kr) from ab initio potentials. *Journal of Chemical Physics*, **2001**, 114, 9919-9928	3.9	35
92	Ab initio study of the nonadditive effects in the trimer of ammonia. *Journal of Chemical Physics*, **1991**, 95, 5169-5178	3.9	35
91	Aurophilic Interactions from Wave Function, Symmetry-Adapted Perturbation Theory, and Rangehybrid Approaches. *Journal of Chemical Theory and Computation*, **2011**, 7, 2399-407	6.4	34
90	Ab initio study of the O2(X 3Σg−)+He(1S) van der Waals cluster. *Journal of Chemical Physics*, **1996**, 104, 7997-8002	3.9	34
89	Studies of dispersion energy in hydrogen-bonded systems. H2O–HOH, H2O–HF, H3N–HF, HF–HF. *Journal of Chemical Physics*, **1984**, 80, 1535-1542	3.9	34
88	Ab initio study of He(1S)+Cl2(X 1Σg+,3Πu) potential energy surfaces. *Journal of Chemical Physics*, **1994**, 101, 6800-6809	3.9	33
87	Effects of external ions on the dynamics of proton transfer across a hydrogen bond. *The Journal of Physical Chemistry*, **1985**, 89, 1835-1840		33
86	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	1.8	32
85	Density functional theory approach to noncovalent interactions via monomer polarization and Pauli blockade. *Physical Review Letters*, **2010**, 104, 163001	7.4	31
84	Ab initio based study of the ArO– photoelectron spectra: Selectivity of spin–orbit transitions. *Journal of Chemical Physics*, **2000**, 112, 5852-5865	3.9	31
83	Ab initio study of nonadditive interactions in the Ar2HF and Ar2HCl clusters. II. Analysis of exchange and induction effects. *Journal of Chemical Physics*, **1994**, 101, 10708-10716	3.9	30
82	Interactions of lanthanide atoms: Comparative ab initio study of YbHe, Yb 2 and TmHe, TmYb potentials. *European Physical Journal D*, **2007**, 45, 147-153	1.3	28

81	Proton□donor properties of water and ammonia in van der Waals complexes with rare-gas atoms. Kr□H2O and Kr□NH3. *Journal of Chemical Physics*, **1992**, 97, 8181-8187	3.9	28
80	Vibrational frequencies and intensities of H-bonded systems. 1:1 and 1:2 complexes of NH3 and PH3 with HF. *Journal of Chemical Physics*, **1987**, 87, 2214-2224	3.9	28
79	Accurate evaluation of SCF and MP2 components of interaction energies. Complexes of HF, OH2, and NH3 with Li+. *Collection of Czechoslovak Chemical Communications*, **1988**, 53, 2214-2229		26
78	Ab initio study of the O2(X 3□□)+Ar(1S) van der Waals interaction. *Journal of Chemical Physics*, **1997**, 106, 7731-7737	3.9	24
77	On the nature of the interaction energy in the Ar-Cl2 complex. *Computational and Theoretical Chemistry*, **1994**, 307, 187-199		24
76	SCF ab initio study of lithium-bonded complexes. *Chemical Physics Letters*, **1980**, 74, 243-247	2.5	24
75	van der Waals interactions and dipole polarizabilities of lanthanides: Tm(2F)-He and Yb(1S)-He potentials. *Journal of Chemical Physics*, **2006**, 124, 114301	3.9	23
74	Ab initio study of the He(1S)+CH(X 2□)interaction. *Journal of Chemical Physics*, **1996**, 105, 9525-9535	3.9	23
73	Comment on □A possible definition of basis set superposition error□*Chemical Physics Letters*, **1995**, 241, 140-145	2.5	23
72	HF-HCl: stationary points on the scf energy hypersurface and thermodynamics of formation. *Chemical Physics Letters*, **1980**, 74, 248-251	2.5	23
71	Electronic structure and spin coupling of the manganese dimer: The state of the art of ab initio approach. *Journal of Chemical Physics*, **2010**, 132, 024312	3.9	22
70	Towards an analytical three-body potential of Ar2Cl□*Journal of Chemical Physics*, **1995**, 103, 299-308	3.9	22
69	On the nature of the interaction energy in the Ar□ClF complex. *Journal of Chemical Physics*, **1993**, 99, 3700-3706	3.9	22
68	Derivation of the supermolecular interaction energy from the monomer densities in the density functional theory. *Chemical Physics Letters*, **2010**, 486, 160-165	2.5	20
67	The effect of two- and three-body interactions in ArnCO2 (n=1,2) on the asymmetric stretching CO2 coordinate: An ab initio study. *Journal of Chemical Physics*, **1997**, 106, 10215-10221	3.9	20
66	Origins and modeling of many-body exchange effects in van der Waals clusters. *Journal of Chemical Physics*, **1997**, 106, 3301-3310	3.9	20
65	Interactions of transition metal atoms with He. *European Physical Journal D*, **2004**, 31, 429-437	1.3	20
64	Ab initio zero electron kinetic energy spectroscopy of the ArCl□and KrCl□anions. *Journal of Chemical Physics*, **2001**, 114, 9929-9937	3.9	20

63	Dynamics of O(3Pj)+Rg collisions on ab initio and scattering potentials. *Journal of Chemical Physics*, **2002**, 116, 1457-1467	3.9	20
62	Studies on the lithium bond. *Chemical Physics Letters*, **1976**, 44, 465-467	2.5	20
61	Density-dependent onset of the long-range exchange: a key to donor-acceptor properties. *Journal of Physical Chemistry A*, **2013**, 117, 11580-6	2.8	18
60	Theoretical vibrational study of the FX???O(CH3)2 hydrogen-bonded complex. *Journal of Chemical Physics*, **1988**, 88, 4861-4866	3.9	18
59	Theoretical studies of lithium bonding in lithium chloride/aliphatic amine complexes. *Chemical Physics*, **1985**, 94, 55-63	2.3	18
58	Range-Separated meta-GGA Functional Designed for Noncovalent Interactions. *Journal of Chemical Theory and Computation*, **2014**, 10, 4297-306	6.4	17
57	Helium atom as a probe of molecular shape and properties: He?H2O complex. *Journal of Molecular Structure*, **1993**, 297, 313-325	3.4	17
56	Contribution of dispersion to the properties of H2S--HF and H2S--HCl. *Journal of Chemical Physics*, **1985**, 83, 1778-1783	3.9	17
55	Properties of strong hydrogen-bonded systems. II. Ab initioSCF-MO study of the hydrogen bond between nitric acid and ammonia. *Journal of Computational Chemistry*, **1980**, 1, 417-419	3.5	17
54	HF-ClF: minima on the 4-31G and 4-31G* energy hypersurfaces and thermodynamics of formation. *Chemical Physics Letters*, **1981**, 82, 469-472	2.5	17
53	Interaction potentials for Br(-)-Rg (Rg=He-Rn): spectroscopy and transport coefficients. *Journal of Chemical Physics*, **2006**, 125, 64305	3.9	16
52	Modeling of adiabatic and diabatic potential energy surfaces of Cl(2P)?H2(1Σ+) prereactive complex from ab initio calculations. *Journal of Chemical Physics*, **2002**, 117, 4709-4719	3.9	16
51	Effect of secondary basis-set superposition error upon calculated vibrational intensities. *Chemical Physics Letters*, **1986**, 131, 230-236	2.5	16
50	Nonadditive interactions in ns2 and spin-polarized ns metal atom trimers. *Journal of Chemical Physics*, **2008**, 129, 134302	3.9	15
49	Ab initio simulations of the KrO⁻ anion photoelectron spectra. *Journal of Chemical Physics*, **2002**, 117, 2629-2634	3.9	15
48	Ab initio long-range interaction and adiabatic channel capture model for ultracold reactions between the KRb molecules. *Journal of Chemical Physics*, **2012**, 137, 114305	3.9	14
47	Ar?C2H2: a challenging system for ab initio calculations. *Journal of Molecular Structure*, **1997**, 436-437, 387-400	3.4	14
46	The methylation effect in amine...HF hydrogen-bonded systems. Quantum chemical and statistical thermodynamic study. *The Journal of Physical Chemistry*, **1984**, 88, 5923-5927		14

45	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	3.8	14
44	The nature of three-body interactions in DFT: Exchange and polarization effects. *Journal of Chemical Physics*, **2017**, 147, 084106	3.9	13
43	Tuned range-separated hybrid functionals in the symmetry-adapted perturbation theory. *Journal of Chemical Physics*, **2014**, 141, 134120	3.9	13
42	Ab initio study of Tm-He interactions and dynamics in a magnetic trap. *Physical Review A*, **2006**, 74,	2.6	13
41	Interactions of transition metal atoms in high-spin states: Cr2, Sc-Cr, and Sc-Kr. *Journal of Chemical Physics*, **2007**, 127, 244302	3.9	13
40	Ab initio calculations on the lithium fluoride□ethylene complex. *Journal of Chemical Physics*, **1977**, 67, 5400-5401	3.9	13
39	Properties of strong hydrogen-bonded systems. *Chemical Physics Letters*, **1980**, 72, 115-118	2.5	12
38	Density functional theory approach to gold-ligand interactions: separating true effects from artifacts. *Journal of Chemical Physics*, **2014**, 140, 244313	3.9	11
37	Ab initio calculations and modeling of three-dimensional adiabatic and diabatic potential energy surfaces of F(2P)□□H2(1□) Van der Waals complex. *International Journal of Quantum Chemistry*, **2002**, 90, 1038-1048	2.1	11
36	Hydrogen bonding of water, hydrogen sulphide and related acceptors with electron donors. *Journal of Molecular Structure*, **1976**, 30, 271-290	3.4	11
35	Europium dimer: van der Waals molecule with extremely weak antiferromagnetic spin coupling. *Journal of Chemical Physics*, **2009**, 131, 241102	3.9	10
34	From Intermolecular Interactions to Incipient Chemical Bond. *Collection of Czechoslovak Chemical Communications*, **1998**, 63, 1473-1484		10
33	Ab initio study of the H2CO□Ar complex. *Journal of Chemical Physics*, **1993**, 99, 5211-5218	3.9	10
32	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, 3662-73	6.4	9
31	Dispersion-free component of non-covalent interaction via mutual polarization of fragment densities. *Journal of Chemical Physics*, **2012**, 136, 204109	3.9	8
30	Characterization of ArnO□clusters from ab initio and diffusion Monte Carlo calculations. *Journal of Chemical Physics*, **2003**, 118, 2748	3.9	8
29	Study of ArO- and ArO via slow photoelectron velocity-map imaging spectroscopy and Ab initio calculations. *Journal of Physical Chemistry A*, **2009**, 113, 4631-8	2.8	7
28	Study of KrO- and KrO via slow photoelectron velocity-map imaging spectroscopy and ab initio calculations. *Journal of Physical Chemistry A*, **2009**, 113, 14439-46	2.8	7

27	Interactions in open-shell clusters: ab initio study of pre-reactive complex O(3P) + HCl. *Journal of Physical Chemistry A*, **2005**, 109, 11484-94	2.8	7
26	Ab Initio Calculations and Modeling of Three-Dimensional Adiabatic and Diabatic Potential Energy Surfaces of Br(2P)H2(1) Pre-Reactive Complex. *Journal of Physical Chemistry A*, **2002**, 106, 7362-7368	2.8	7
25	Structure and energetics of ArnNOclusters from ab initio calculations. *Journal of Chemical Physics*, **2000**, 112, 10895-10904	3.9	7
24	Search for simplified procedure for the evaluation of the Gibbs free energy of hydrogen-bond formation. *The Journal of Physical Chemistry*, **1983**, 87, 2608-2614		7
23	A first-principles-based correlation functional for harmonious connection of short-range correlation and long-range dispersion. *Journal of Chemical Physics*, **2012**, 137, 204121	3.9	6
22	Ab initio study of the Br(2P)-HBr van der Waals complex. *Journal of Chemical Physics*, **2009**, 130, 184304	3.9	6
21	Many-body exchange effects in clusters of rare gases with a chromophore: He2CO2. *Chemical Physics*, **1998**, 239, 573-591	2.3	6
20	Modeling of the three-body effects in the Ar2Otrimer from ab initio calculations. *Journal of Chemical Physics*, **2003**, 118, 2731	3.9	6
19	Anisotropy of correlation effects in hydrogen-bonded systems: the HF dimer. *Chemical Physics Letters*, **1989**, 161, 532-538	2.5	6
18	On the Nature of Luminescence Thermochromism of Multinuclear Copper(I) Benzoate Complexes in the Crystalline State. *Crystals*, **2019**, 9, 36	2.3	5
17	A density functional theory approach to noncovalent interactions via interacting monomer densities. *Physical Chemistry Chemical Physics*, **2010**, 12, 14686-92	3.6	5
16	Interactions and collisions of cold metal atoms in magnetic traps. *Physica Scripta*, **2009**, 80, 048109	2.6	5
15	Ab initio study of van der Waals interaction of formamide with a nonpolar partner. Ar???H2NCOH complex. *Journal of Chemical Physics*, **1996**, 105, 8213-8222	3.9	5
14	Noncovalent interactions determine the conformation of aurophilic complexes with 2-mercapto-4-methyl-5-thiazoleacetic acid ligands. *Dalton Transactions*, **2015**, 44, 13641-50	4.3	4
13	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	3.9	4
12	Ab Initio Study of Nonadditive Effects in the (H2O)2H2 Cluster. *The Journal of Physical Chemistry*, **1996**, 100, 10875-10881		4
11	Theoretical prediction of the ArOanion ZEKE photoelectron spectrum. *Chemical Physics Letters*, **2001**, 347, 415-420	2.5	4
10	Proton-donor properties of water and ammonia in van der Waals complexes. BeH2O and BeNH3. *Journal of Chemical Physics*, **1993**, 98, 7020-7028	3.9	4

9	Assessment of SAPT(DFT) with meta-GGA functionals. *Journal of Molecular Modeling*, **2020**, 26, 102	2	3
8	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	2.3	3
7	Structures and energies of the lithiated silanes. *Journal of the Chemical Society Perkin Transactions II*, **1989**, 131-135		3
6	Nonadditivity of the SCF interaction energy in the (LiH)3 complex. *International Journal of Quantum Chemistry*, **1980**, 17, 1069-1074	2.1	3
5	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		2
4	Reassessing the Role of Holes in Noncovalent Interactions: It is Pauli Repulsion that Counts.. *Frontiers in Chemistry*, **2022**, 10, 858946	5	2
3	Water Soluble Host–Guest Chemistry Involving Aromatic N-Oxides and Sulfonateresorcinarene. *Symmetry*, **2020**, 12, 1751	2.7	1
2	The nature of Van der Waals bond. *Theoretical and Computational Chemistry*, **1999**, 6, 665-699		1
1	Ab initio calculations and modeling of three-body forces in Ar2H2O. *International Journal of Quantum Chemistry*, **2002**, 90, 1215-1231	2.1	