Mariusz KÅ‚obukowski

List of Publications by Year
in descending order

54 papers	1,459 citations	304743 22 h-index	315739 38 g-index
54 all docs	54 docs citations	54 times ranked	1281 citing authors

#	Article	IF	Citations
1	The effects of ring strain on cyclic tetraaryl[5]cumulenes. Chemistry - A European Journal, 2022, , .	3.3	0
2	Computational Prediction and Experimental Validation of the Unique Molecular Mode of Action of Scoulerine. Molecules, 2022, 27, 3991.	3.8	2
3	Structure, reactions, and electronic spectra of the rare gas cyanohydrides and isocyanohydrides, HRgCN and HRgNC (Rg = Xe or Rn). Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 245102.	1.5	0
4	Mechanochemical synthesis of 0D and 3D cesium lead mixed halide perovskites. Chemical Communications, 2019, 55, 5079-5082.	4.1	78
5	Computational study of the electronic spectra of the rare gas fluorohydrides HRgF (Rg = Ar, Kr, Xe,) Tj ETQq1 1 0.784314 rgBT /Overlock	1.5	1
6	Multireference Methods for Calculating the Dissociation Enthalpy of Tetrahedral P4 to Two P2. Journal of Physical Chemistry A, 2018, 122, 5742-5749.	2.5	8
7	Engaging dual donor sites within an N-heterocyclic olefin phosphine ligand. Dalton Transactions, 2017, 46, 5946-5954.	3.3	9
8	Anesthetic Alterations of Collective Terahertz Oscillations in Tubulin Correlate with Clinical Potency: Implications for Anesthetic Action and Post-Operative Cognitive Dysfunction. Scientific Reports, 2017, 7, 9877.	3.3	43
9	Hydrogen bonding and autoionization in confined bifluoride system FHFâ¯. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 155101.	1.5	2
10	Explaining the Microtubule Energy Balance: Contributions Due to Dipole Moments, Charges, van der Waals and Solvation Energy. International Journal of Molecular Sciences, 2017, 18, 2042.	4.1	7
11	Antitumor Activity of Lankacidin Group Antibiotics Is Due to Microtubule Stabilization via a Paclitaxel-like Mechanism. Journal of Medicinal Chemistry, 2016, 59, 9532-9540.	6.4	23
12	Analysis of the binding mode of laulimalide to microtubules: Establishing a laulimalideâ€“tubulin pharmacophore. Journal of Biomolecular Structure and Dynamics, 2016, 34, 1455-1469.	3.5	16
13	Elucidating the Mechanism of Action of the Clinically Approved Taxanes: A Comprehensive Comparison of Local and Allosteric Effects. Chemical Biology and Drug Design, 2015, 86, 1253-1266.	3.2	22
14	Detailed Per-residue Energetic Analysis Explains the Driving Force for Microtubule Disassembly. PLoS Computational Biology, 2015, 11, e1004313.	3.2	22
15	The Unique Binding Mode of Laulimalide to Two Tubulin Protofilaments. Chemical Biology and Drug Design, 2015, 86, 190-199.	3.2	27
16	Comparison of xenon and radon metal halides. Chemical Physics Letters, 2015, 638, 249-252.	2.6	2
17	Designing and Testing of Novel Taxanes to Probe the Highly Complex Mechanisms by Which Taxanes Bind to Microtubules and Cause Cytotoxicity to Cancer Cells. PLoS ONE, 2015, 10, e0129168.	2.5	11
18	Analysis of the Strength of Interfacial Hydrogen Bonds between Tubulin Dimers Using Quantum Theory of Atoms in Molecules. Biophysical Journal, 2014, 107, 740-750.	0.5	45

#	Article	IF	Citations
19	Estimating hydrogen bond energies: comparison of methods. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	23
20	Structure and stability of organic molecules containing heavy rare gas atoms. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	13
21	Basis set effects in simple compounds of heavy rare gases. Canadian Journal of Chemistry, 2013, 91, 894-901.	1.1	2
22	Interactions of laulimalide, peloruside, and their derivatives with the isoforms of Î²-tubulin. Canadian Journal of Chemistry, 2013, 91, 511-517.	1.1	13
23	Natural Spinors Reveal How the Spinâ€“Orbit Coupling Affects the Jahnâ€“Teller Distortions in the Hexafluorotungstate(V) Anion. Journal of Chemical Theory and Computation, 2012, 8, 3061-3071.	5.3	12
24	Relativistic study of tautomerism and core electron binding energies of thio- and selenocytosine. Structural Chemistry, 2012, 23, 1293-1299.	2.0	5
25	Effects of Spinâ€“Orbit Coupling on Covalent Bonding and the Jahnâ€“Teller Effect Are Revealed with the Natural Language of Spinors. Journal of Chemical Theory and Computation, 2011, 7, 2864-2875.	5.3	37
26	New parameterization of the PM3 method for monosaccharides. Chemical Physics Letters, 2010, 500, 140-143.	2.6	5
27	Model core potentials of p-block elements generated considering the Douglasâ€“Kroll relativistic effects, suitable for accurate spin-orbit coupling calculations. Journal of Chemical Physics, 2010, 133, 114107.	3.0	21
28	Model Core Potential and All-Electron Studies of Molecules Containing Rare Gas Atoms^{â€}. Journal of Physical Chemistry A, 2010, 114, 8786-8792.	2.5	11
29	Calibration of new model core potentials for main group elements. International Journal of Quantum Chemistry, 2009, 109, 3235-3245.	2.0	4
30	DFT studies of complexes between ethylenediamine tetraacetate and alkali and alkaline earth cations. Canadian Journal of Chemistry, 2009, 87, 1492-1498.	1.1	5
31	Relativistic calculations on the ground and excited states of AgH and AuH in cylindrical harmonic confinement. Theoretical Chemistry Accounts, 2007, 118, 607-622.	1.4	11
32	Perturbation theory of the spatial confinement effects in the Rydberg HeH molecule. Chemical Physics Letters, 2006, 422, 391-396.	2.6	5
33	Compact and efficient basis sets of s- and p-block elements for model core potential method. Journal of Chemical Physics, 2005, 122, 074104.	3.0	65
34	Configuration interaction calculations on beryllium molecular ion in cylindrical harmonic confining potential. Molecular Physics, 2005, 103, 2599-2612.	1.7	6
35	Low-Lying Excited States of the Hydrogen Molecule in Cylindrical Harmonic Confinement. Advances in Quantum Chemistry, 2005, 48, 59-89.	0.8	34
36	The well-tempered model core potentials for the main-group elements Li?Rn. Theoretical Chemistry Accounts, 2004, 112, 33-39.	1.4	7

#	Article	IF	Citations
37	Improved model core potentials for the second- and third-row transition metals. Journal of Computational Chemistry, 2004, 25, 1206-1213.	3.3	28
38	MCQDPT studies of beryllium molecule in cylindrical harmonic confining potential. Molecular Physics, 2004, 102, 2511-2519.	1.7	6
39	Development of new pseudopotential methods: Improved model core potentials for the first-row transition metals. Journal of Computational Chemistry, 2003, 24, 1009-1015.	3.3	35
40	Improved model core potentials: Application to the thermochemistry of organoxenon complexes. International Journal of Quantum Chemistry, 2002, 90, 1099-1107.	2.0	18
41	Quantum chemistry of confined systems: structure and vibronic spectra of a confined hydrogen molecule. Chemical Physics Letters, 2001, 349, 215-219.	2.6	66
42	Well-tempered model core potentials for groups 17 and 18. Computational and Theoretical Chemistry, 2001, 547, 163-170.	1.5	5
43	New Zirconium Hydrocarbyl Bis(phosphoranimino) â€œPincerâ€•Carbene Complexes. Organometallics, 1999, 18, 4226-4229.	2.3	100
44	Model Core Potentials: Theory and Applications. Computational Chemistry - Reviews of Current Trends, 1999, , 49-74.	0.4	30
45	Model potentials for main group elements Li through Rn. Journal of Chemical Physics, 1997, 106, 8084-8092.	3.0	71
46	A Contribution to the Understanding of Carbonyl Migration in Mn2(CO)10via the Pairwise Exchange Mechanism. Journal of Physical Chemistry A, 1997, 101, 8734-8740.	2.5	26
47	Structure and Reactions of the Succinimidyl Radical:â€‰ A Density Functional Study. Journal of the American Chemical Society, 1997, 119, 3339-3346.	13.7	8
48	Ab initio SCF and Mï¿½ller?plesset studies on hexafluorides of selenium and tellurium. Journal of Computational Chemistry, 1993, 14, 1234-1239.	3.3	10
49	Model potentials for molecular calculations. I. The sdâ€MP set for transition metal atoms Sc through Hg. Journal of Computational Chemistry, 1987, 8, 226-255.	3.3	103
50	Model potentials for molecular calculations. II. The spdâ€MP set for transition metal atoms Sc through Hg. Journal of Computational Chemistry, 1987, 8, 256-264.	3.3	84
51	Nonempirical self-consistent modified extended Huckel calculations on heavy-metal systems. II. Electronic structure, bonding, and spectra of the binuclear Pt2(P2O5H2)44? ion. International Journal of Quantum Chemistry, 1986, 30, 239-252.	2.0	15
52	Model potential study of the interactions in Ar2, Kr2 and Xe2 dimers. Molecular Physics, 1984, 52, 1495-1513.	1.7	56
53	Compact contracted Gaussian-type basis sets for halogen atoms. Basis-set superposition effects on molecular properties. Journal of Computational Chemistry, 1984, 5, 146-161.	3.3	86
54	Model potential method in molecular calculations. The Journal of Physical Chemistry, 1984, 88, 4880-4886.	2.9	115