

Mariusz KÅ,obukowski

List of Publications by Year in descending order

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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	Model potential method in molecular calculations. The Journal of Physical Chemistry, 1984, 88, 4880-4886.	2.9	115
2	Model potentials for molecular calculations. I. The <i>sd</i> -EMP set for transition metal atoms Sc through Hg. Journal of Computational Chemistry, 1987, 8, 226-255.	3.3	103
3	New Zirconium Hydrocarbyl Bis(phosphoranimino) Pincer-Carbene Complexes. Organometallics, 1999, 18, 4226-4229.	2.3	100
4	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
5	Model potentials for molecular calculations. II. The <i>spd</i> -EMP set for transition metal atoms Sc through Hg. Journal of Computational Chemistry, 1987, 8, 256-264.	3.3	84
6	Mechanochemical synthesis of 0D and 3D cesium lead mixed halide perovskites. Chemical Communications, 2019, 55, 5079-5082.	4.1	78
7	Model potentials for main group elements Li through Rn. Journal of Chemical Physics, 1997, 106, 8084-8092.	3.0	71
8	Quantum chemistry of confined systems: structure and vibronic spectra of a confined hydrogen molecule. Chemical Physics Letters, 2001, 349, 215-219.	2.6	66
9	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
10	Model potential study of the interactions in Ar ₂ , Kr ₂ and Xe ₂ dimers. Molecular Physics, 1984, 52, 1495-1513.	1.7	56
11	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
12	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
13	Effects of Spin-Orbit Coupling on Covalent Bonding and the Jahn-Teller Effect Are Revealed with the Natural Language of Spinors. Journal of Chemical Theory and Computation, 2011, 7, 2864-2875.	5.3	37
14	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
15	Low-Lying Excited States of the Hydrogen Molecule in Cylindrical Harmonic Confinement. Advances in Quantum Chemistry, 2005, 48, 59-89.	0.8	34
16	Model Core Potentials: Theory and Applications. Computational Chemistry - Reviews of Current Trends, 1999, , 49-74.	0.4	30
17	Improved model core potentials for the second- and third-row transition metals. Journal of Computational Chemistry, 2004, 25, 1206-1213.	3.3	28
18	The Unique Binding Mode of Lauimalide to Two Tubulin Protofilaments. Chemical Biology and Drug Design, 2015, 86, 190-199.	3.2	27

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19	A Contribution to the Understanding of Carbonyl Migration in Mn ₂ (CO) ₁₀ via the Pairwise Exchange Mechanism. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8734-8740.	2.5	26
20	Estimating hydrogen bond energies: comparison of methods. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	23
21	Antitumor Activity of Lankacidin Group Antibiotics Is Due to Microtubule Stabilization via a Paclitaxel-like Mechanism. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 9532-9540.	6.4	23
22	Elucidating the Mechanism of Action of the Clinically Approved Taxanes: A Comprehensive Comparison of Local and Allosteric Effects. <i>Chemical Biology and Drug Design</i> , 2015, 86, 1253-1266.	3.2	22
23	Detailed Per-residue Energetic Analysis Explains the Driving Force for Microtubule Disassembly. <i>PLoS Computational Biology</i> , 2015, 11, e1004313.	3.2	22
24	Model core potentials of p-block elements generated considering the Douglas-Kroll relativistic effects, suitable for accurate spin-orbit coupling calculations. <i>Journal of Chemical Physics</i> , 2010, 133, 114107.	3.0	21
25	Improved model core potentials: Application to the thermochemistry of organoxenon complexes. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 1099-1107.	2.0	18
26	Analysis of the binding mode of laulimalide to microtubules: Establishing a laulimalide-tubulin pharmacophore. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 1455-1469.	3.5	16
27	Nonempirical self-consistent modified extended Huckel calculations on heavy-metal systems. II. Electronic structure, bonding, and spectra of the binuclear Pt ₂ (P ₂ O ₅ H ₂) ₄ ⁴⁺ ion. <i>International Journal of Quantum Chemistry</i> , 1986, 30, 239-252.	2.0	15
28	Structure and stability of organic molecules containing heavy rare gas atoms. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	1.4	13
29	Interactions of laulimalide, peloruside, and their derivatives with the isoforms of β -tubulin. <i>Canadian Journal of Chemistry</i> , 2013, 91, 511-517.	1.1	13
30	Natural Spinors Reveal How the Spin-Orbit Coupling Affects the Jahn-Teller Distortions in the Hexafluorotungstate(V) Anion. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3061-3071.	5.3	12
31	Relativistic calculations on the ground and excited states of AgH and AuH in cylindrical harmonic confinement. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 607-622.	1.4	11
32	Model Core Potential and All-Electron Studies of Molecules Containing Rare Gas Atoms ^{<sup>>} . <i>Journal of Physical Chemistry A</i> , 2010, 114, 8786-8792.	2.5	11
33	Designing and Testing of Novel Taxanes to Probe the Highly Complex Mechanisms by Which Taxanes Bind to Microtubules and Cause Cytotoxicity to Cancer Cells. <i>PLoS ONE</i> , 2015, 10, e0129168.	2.5	11
34	Ab initio SCF and Møller-Plesset studies on hexafluorides of selenium and tellurium. <i>Journal of Computational Chemistry</i> , 1993, 14, 1234-1239.	3.3	10
35	Engaging dual donor sites within an N-heterocyclic olefin phosphine ligand. <i>Dalton Transactions</i> , 2017, 46, 5946-5954.	3.3	9
36	Structure and Reactions of the Succinimidyl Radical: A Density Functional Study. <i>Journal of the American Chemical Society</i> , 1997, 119, 3339-3346.	13.7	8

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37	Multireference Methods for Calculating the Dissociation Enthalpy of Tetrahedral P ₄ to Two P ₂ . <i>Journal of Physical Chemistry A</i> , 2018, 122, 5742-5749.	2.5	8
38	The well-tempered model core potentials for the main-group elements Li?Rn. <i>Theoretical Chemistry Accounts</i> , 2004, 112, 33-39.	1.4	7
39	Explaining the Microtubule Energy Balance: Contributions Due to Dipole Moments, Charges, van der Waals and Solvation Energy. <i>International Journal of Molecular Sciences</i> , 2017, 18, 2042.	4.1	7
40	MCQDPT studies of beryllium molecule in cylindrical harmonic confining potential. <i>Molecular Physics</i> , 2004, 102, 2511-2519.	1.7	6
41	Configuration interaction calculations on beryllium molecular ion in cylindrical harmonic confining potential. <i>Molecular Physics</i> , 2005, 103, 2599-2612.	1.7	6
42	Well-tempered model core potentials for groups 17 and 18. <i>Computational and Theoretical Chemistry</i> , 2001, 547, 163-170.	1.5	5
43	Perturbation theory of the spatial confinement effects in the Rydberg HeH molecule. <i>Chemical Physics Letters</i> , 2006, 422, 391-396.	2.6	5
44	DFT studies of complexes between ethylenediamine tetraacetate and alkali and alkaline earth cations. <i>Canadian Journal of Chemistry</i> , 2009, 87, 1492-1498.	1.1	5
45	New parameterization of the PM3 method for monosaccharides. <i>Chemical Physics Letters</i> , 2010, 500, 140-143.	2.6	5
46	Relativistic study of tautomerism and core electron binding energies of thio- and selenocytosine. <i>Structural Chemistry</i> , 2012, 23, 1293-1299.	2.0	5
47	Calibration of new model core potentials for main group elements. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 3235-3245.	2.0	4
48	Basis set effects in simple compounds of heavy rare gases. <i>Canadian Journal of Chemistry</i> , 2013, 91, 894-901.	1.1	2
49	Comparison of xenon and radon metal halides. <i>Chemical Physics Letters</i> , 2015, 638, 249-252.	2.6	2
50	Hydrogen bonding and autoionization in confined bifluoride system FHF ⁻ . <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2017, 50, 155101.	1.5	2
51	Computational Prediction and Experimental Validation of the Unique Molecular Mode of Action of Scoulerine. <i>Molecules</i> , 2022, 27, 3991.	3.8	2
52	Computational study of the electronic spectra of the rare gas fluorohydrides HRgF (Rg = Ar, Kr, Xe,) Tj ETQq0 0 0 rgBT /Overlqck 10 Tf 5	1.5	1
53	Structure, reactions, and electronic spectra of the rare gas cyanohydrides and isocyanohydrides, HRgCN and HRgNC (Rg = Xe or Rn). <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2020, 53, 245102.	1.5	0
54	The effects of ring strain on cyclic tetraaryl[5]cumulenes. <i>Chemistry - A European Journal</i> , 2022, , .	3.3	0