

Szczepan Roszak

List of Publications by Year in descending order

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24
papers

200
citations

1040056

9
h-index

1058476

14
g-index

25
all docs

25
docs citations

25
times ranked

295
citing authors

#	ARTICLE	IF	CITATIONS
1	First-Principles Modeling of Non-covalent Interactions in Molecular Systems and Extended Materials. , 2022, , 71-124.		0
2	The hybrid models, containing hydrolytic and electron-driven processes, in theoretical study of oxaliplatin biotransformation. Journal of Molecular Modeling, 2020, 26, 286.	1.8	1
3	NMR studies of daidzein and puerarin: active anti-oxidants in traditional Chinese medicine. Journal of Molecular Modeling, 2019, 25, 202.	1.8	16
4	NMR measurements and DFT studies of nuclear magnetic shielding in emodin and chuanxiongazine molecules. Journal of Molecular Structure, 2018, 1166, 304-310.	3.6	9
5	In silico modeling of functionalized graphene oxide-metal cluster conjugates as Raman probe: Raman activity of pyridine. Structural Chemistry, 2017, 28, 379-389.	2.0	2
6	Comparative study of hydrolytic and electron-driven processes in carboplatin biotransformation. Journal of Inorganic Biochemistry, 2017, 170, 148-159.	3.5	9
7	Understanding the influence of low-frequency vibrations on the hydrogen bonds of acetic acid and acetamide dimers. Physical Chemistry Chemical Physics, 2017, 19, 24866-24878.	2.8	10
8	Synthesis and Electrochromic Properties of Conducting Polymers Based on Highly Planar 2,7-disubstituted Xanthene Derivatives. ChemPlusChem, 2015, 80, 679-687.	2.8	4
9	Structure of the hexagonal NaYF ₄ phase from first-principles molecular dynamics. RSC Advances, 2014, 4, 22526.	3.6	26
10	Role of the Multipolar Electrostatic Interaction Energy Components in Strong and Weak Cation-π Interactions. Journal of Physical Chemistry A, 2013, 117, 7989-8000.	2.5	12
11	Exploring Relative Thermodynamic Stabilities of Formic Acid and Formamide Dimers – Role of Low-Frequency Hydrogen-Bond Vibrations. Journal of Chemical Theory and Computation, 2013, 9, 1016-1026.	5.3	17
12	The theoretical studies of interactions of the OH ⁺ (H ₂ O) _n clusters evolution toward the hydroxide anion hydration. International Journal of Quantum Chemistry, 2012, 112, 3046-3051.	2.0	3
13	Theoretical studies on the structure and electronic properties of cubic gold nanoclusters. Canadian Journal of Chemical Engineering, 2012, 90, 852-859.	1.7	4
14	Effects of two vibrational modes in the dissociative electron attachment to CF_3 . Physical Review A, 2009, 79, .	2.5	14
15	Functionalized Phenothiazine and Carbazole Chromophores: Synthesis and Characterization. Phosphorus, Sulfur and Silicon and the Related Elements, 2009, 184, 1257-1268.	1.6	0
16	The chemistry of lithium-modified carbonium cations. Molecular Physics, 2005, 103, 2215-2222.	1.7	0
17	Clusters, the intermediate state of matter. Theoretical and Computational Chemistry, 2004, 15, 67-84.	0.4	3
18	Ab initio study of dissolution reactions of five-membered aluminosilicate framework rings. International Journal of Quantum Chemistry, 2004, 96, 365-373.	2.0	8

#	ARTICLE	IF	CITATIONS
19	Studies of metal isotope and deuteration effects in vibrational spectra of palladium(II) complex with histamine. <i>International Journal of Quantum Chemistry</i> , 2004, 96, 355-364.	2.0	5
20	Quantum Chemical Studies of Neutral and Ionized DyX, DyX ₂ , and DyX ₃ Species (X = F, Cl, Br, I) and the Implications for the Mass Spectra of Gaseous DyX ₃ . <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 1212-1218.	2.0	11
21	Ab Initio Studies of the Microsolvation of Ions. <i>Journal of Physical Chemistry A</i> , 2003, 107, 949-955.	2.5	26
22	The structures and properties of cis- and trans-MeCl ₂ (NH ₃) ₂ , Me=Pd and Pt complexes, in ground and excited states. <i>International Journal of Quantum Chemistry</i> , 2001, 83, 213-219.	2.0	8
23	Ionic Clusters with Weakly Interacting Components-Magic Numbers Rationalized by the Shell Structure. <i>Computational Chemistry - Reviews of Current Trends</i> , 2001, , 179-196.	0.4	2
24	Structure and Nature of the Interaction of the CH ₃ N ₂ ⁺ Ion Shellvated by H ₂ Molecules: \hat{A} CH ₃ N ₂ ⁺ (H ₂) _{n=1-9} . <i>Journal of Physical Chemistry A</i> , 1999, 103, 9138-9143.	2.5	8