Szczepan Roszak

List of Publications by Year
in descending order

24	200	1040056 9	1058476 14
papers	citations	h-index	g-index

25	25	25	295
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ab Initio Studies of the Microsolvation of Ions. Journal of Physical Chemistry A, 2003, 107, 949-955.	2.5	26
2	Structure of the hexagonal NaYF4 phase from first-principles molecular dynamics. RSC Advances, 2014, 4, 22526.	3.6	26
3	Exploring Relative Thermodynamic Stabilities of Formic Acid and Formamide Dimers â€“ Role of Low-Frequency Hydrogen-Bond Vibrations. Journal of Chemical Theory and Computation, 2013, 9, 1016-1026.	5.3	17
4	NMR studies of daidzein and puerarin: active anti-oxidants in traditional Chinese medicine. Journal of Molecular Modeling, 2019, 25, 202.	1.8	16
5	Effects of two vibrational modes in the dissociative electron attachment to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CF</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:m Physical Review A, 2009, 79, .	2.5	14
6	Role of the Multipolar Electrostatic Interaction Energy Components in Strong and Weak Cationâ^'Ï€ Interactions. Journal of Physical Chemistry A, 2013, 117, 7989-8000.	2.5	12
7	Quantum Chemical Studies of Neutral and Ionized DyX, DyX2, and DyX3 Species (X = F, Cl, Br, I) and the Implications for the Mass Spectra of Gaseous DyX3. European Journal of Inorganic Chemistry, 2004, 2004, 1212-1218.	2.0	11
8	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
9	Comparative study of hydrolytic and electron-driven processes in carboplatin biotransformation. Journal of Inorganic Biochemistry, 2017, 170, 148-159.	3.5	9
10	NMR measurements and DFT studies of nuclear magnetic shielding in emodin and chuanxiongzine molecules. Journal of Molecular Structure, 2018, 1166, 304-310.	3.6	9
11	Structure and Nature of the Interaction of the CH3N2+Ion Shellvated by H2Molecules:Â CH3N2+(H2)n=1-9. Journal of Physical Chemistry A, 1999, 103, 9138-9143.	2.5	8
12	The structures and properties ofcis- andtrans-MeCl2(NH3)2, Me=Pd and Pt complexes, in ground and excited states. International Journal of Quantum Chemistry, 2001, 83, 213-219.	2.0	8
13	Ab initio study of dissolution reactions of five-membered aluminosilicate framework rings. International Journal of Quantum Chemistry, 2004, 96, 365-373.	2.0	8
14	Studies of metal isotope and deuteration effects in vibrational spectra of palladium(II) complex with histamine. International Journal of Quantum Chemistry, 2004, 96, 355-364.	2.0	5
15	Theoretical studies on the structure and electronic properties of cubic gold nanoclusters. Canadian Journal of Chemical Engineering, 2012, 90, 852-859.	1.7	4
16	Synthesis and Electrochromic Properties of Conducting Polymers Based on Highly Planar 2,7â€Đisubstituted Xanthene Derivatives. ChemPlusChem, 2015, 80, 679-687.	2.8	4
17	Clusters, the intermediate state of matter. Theoretical and Computational Chemistry, 2004, 15, 67-84.	0.4	3
18	The theoretical studies of interactions of the OH^{â^'}(H₂O)_n clusters evolution toward the hydroxide anion hydration. International Journal of Quantum Chemistry, 2012, 112, 3046-3051.	2.0	3

#	Article	IF	Citations
19	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
20	Ionic Clusters with Weakly Interacting Components-Magic Numbers Rationalized by the Shell Structure. Computational Chemistry - Reviews of Current Trends, 2001, , 179-196.	0.4	2
21	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
22	The chemistry of lithium-modified carbonium cations. Molecular Physics, 2005, 103, 2215-2222.	1.7	0
23	Functionalized Phenothiazine and Carbazole Chromophores: Synthesis and Characterization. Phosphorus, Sulfur and Silicon and the Related Elements, 2009, 184, 1257-1268.	1.6	0
24	First-Principles Modeling of Non-covalent Interactions in Molecular Systems and Extended Materials. , 2022, , 71-124.		0