MaÅ‚gorzata Witko

List of Publications by Year
in descending order

44 papers	896 citations	361045 20 h-index	500791 28 g-index
49 all docs	49 docs citations	49 times ranked	1156 citing authors

#	Article	IF	Citations
1	Tungsten and Molybdenum Heteropolyanions with Different Central Ionsâ€"Correlation between Theory and Experiment. Molecules, 2022, 27, 187.	1.7	2
2	Functionalized tricalcium phosphate and poly(3-hydroxyoctanoate) derived composite scaffolds as platforms for the controlled release of diclofenac. Ceramics International, 2021, 47, 3876-3883.	2.3	13
3	Comparison of Catalytic Properties of Vanadium Centers Introduced into BEA Zeolite and Present on (010) V2O5 Surfaceâ€"DFT Studies. Catalysts, 2020, 10, 1080.	1.6	3
4	Physicochemical and Biological Characterisation of Diclofenac Oligomeric Poly(3-hydroxyoctanoate) Hybrids as Î²-TCP Ceramics Modifiers for Bone Tissue Regeneration. International Journal of Molecular Sciences, 2020, 21, 9452.	1.8	11
5	Novel bioresorbable tricalcium phosphate/polyhydroxyoctanoate (TCP/PHO) composites as scaffolds for bone tissue engineering applications. Journal of the Mechanical Behavior of Biomedical Materials, 2019, 98, 235-245.	1.5	20
6	Polyhydroxyalkanoate-derived hydrogen-bond donors for the synthesis of new deep eutectic solvents. Green Chemistry, 2019, 21, 3116-3126.	4.6	29
7	Structural, topographical, and mechanical characteristics of purified polyhydroxyoctanoate polymer. Journal of Applied Polymer Science, 2019, 136, 47192.	1.3	28
8	Effect of cobalt location in Keggin-type heteropoly catalysts on aerobic oxidation of cyclooctane: Experimental and theoretical study. Applied Catalysis A: General, 2017, 542, 317-326.	2.2	26
9	Factors controlling the reactivity of divalent metal ions towards pheophytin a. Journal of Biological Inorganic Chemistry, 2017, 22, 941-952.	1.1	9
10	The Influence of Structural Parameters on the Reactivity of Model Complexes for Compound II: A Mini Review. Topics in Catalysis, 2014, 57, 946-952.	1.3	4
11	Mechanistic Insight into Peroxoâ€Shunt Formation of Biomimetic Models for Compoundâ€...II, Their Reactivity toward Organic Substrates, and the Influence of Nâ€Methylimidazole Axial Ligation. Chemistry - A European Journal, 2014, 20, 2328-2343.	1.7	17
12	Mechanistic basis for the enantioselectivity of the anaerobic hydroxylation of alkylaromatic compounds by ethylbenzene dehydrogenase. Journal of Inorganic Biochemistry, 2014, 139, 9-20.	1.5	36
13	Metallobacteriochlorophylls as potential dual agents for photodynamic therapy and chemotherapy. Journal of Molecular Modeling, 2013, 19, 4155-4161.	0.8	7
14	Ligation of water to magnesium chelates of biological importance. Journal of Molecular Modeling, 2013, 19, 4661-4667.	0.8	21
15	Hydrogen peroxide as oxidant in bio-mimetic catalysis by manganese porphyrin: Theoretical DFT studies. Canadian Journal of Chemistry, 2013, 91, 642-647.	0.6	5
16	The reaction mechanism of chiral hydroxylation of p-OH and p-NH₂ substituted compounds by ethylbenzene dehydrogenase. Canadian Journal of Chemistry, 2013, 91, 775-786.	0.6	12
17	Ammonium adsorption on BrÃ¸nsted acidic centers on low-index vanadium pentoxide surfaces. Journal of Molecular Modeling, 2013, 19, 4487-4501.	0.8	12
18	Nanospace constraints in mesoporous silica carriersâ€"A factor of critical importance in promoting the catalytic activity of supported ruthenium (II) complex with hemilabile phosphine ligand. Applied Catalysis A: General, 2012, 427-428, 16-23.	2.2	1

#	Article	IF	Citations
19	Allylic oxidation of cyclohexene catalyzed by manganese porphyrins: DFT studies. Catalysis Today, 2011, 169, 10-15.	2.2	14
20	Electronic structure of MoO2. DFT periodic and cluster model studies. Applied Catalysis A: General, 2011, 391, 137-143.	2.2	30
21	Relative stability of low-index V₂O₅surfaces: a density functional investigation. Journal of Physics Condensed Matter, 2009, 21, 095008.	0.7	27
22	Oxygen vacancy formation on clean and hydroxylated low-index<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>V</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mtext> A density functional investigation. Physical Review B, 2009, 79, .	1.1	39
23	Ligand binding properties of cobalamins. Theoretical Chemistry Accounts, 2008, 120, 411-419.	0.5	5
24	How to select an optimal neural model of chemical reactivity?. Neurocomputing, 2008, 72, 241-256.	3.5	23
25	Influence of Anatase Support on Geometrical Structure of Vanadium Oxide at Varying Temperatures and Pressures. Periodic DFT Study. Journal of Physical Chemistry C, 2007, 111, 4216-4225.	1.5	18
26	Quantum Chemical Description of Oxygen Activation Process on Co, Mn, and Mo Porphyrins. Journal of Chemical Theory and Computation, 2007, 3, 914-920.	2.3	22
27	Theoretical density functional theory studies on interactions of small biologically active molecules with isolated heme group. Journal of Computational Chemistry, 2007, 28, 825-831.	1.5	11
28	Sixth International Symposium. Applied Surface Science, 2007, 253, 5565-5569.	3.1	14
29	From activation of dioxygen to formation of high-valent oxo species: Ab initio DFT studies. Journal of Molecular Catalysis A, 2007, 275, 113-120.	4.8	12
30	Application of artificial neural networks and DFT-based parameters for prediction of reaction kinetics of ethylbenzene dehydrogenase. Journal of Computer-Aided Molecular Design, 2006, 20, 145-157.	1.3	37
31	Following natureâ€"Theoretical studies on factors modulating catalytic activity of porphyrins. Journal of Molecular Catalysis A, 2006, 258, 376-380.	4.8	22
32	Reduction and re-oxidation of molybdena and vanadia: DFT cluster model studies. Catalysis Today, 2005, 99, 241-253.	2.2	36
33	Application of the DFT Theory to Study Cobalamin Complexes. Structural Chemistry, 2004, 15, 431-435.	1.0	17
34	Surface oxygen in catalysts based on transition metal oxides. Catalysis Today, 2004, 91-92, 171-176.	2.2	29
35	Oxygen Sites at Molybdena and Vanadia Surfaces: Energetics of the Re-Oxidation Process. Collection of Czechoslovak Chemical Communications, 2004, 69, 121-140.	1.0	9
36	Chemical nature of point defects at the (VO) 2 P 2 O 7 (100) surface. Surface Science, 2003, 538, 160-170.	0.8	8

#	ARTICLE	IF	CITATIONS
37	Reactions of the [Fe(CN)5NO]2â^'complex with biologically relevant thiols. New Journal of Chemistry, 2002, 26, 1495-1502.	1.4	42
38	Nitrite binding to metmyoglobin and methemoglobin in comparison to nitric oxide binding. Journal of Biological Inorganic Chemistry, 2002, 7, 165-176.	1.1	49
39	Surface Cluster Models for V2O5 - Studies of the Importance of Local Geometry. Collection of Czechoslovak Chemical Communications, 1998, 63, 1355-1367.	1.0	5
40	Quantum-chemical description of the active sites for the selective oxidation of hydrocarbons. Catalysis Today, 1996, 32, 89-95.	2.2	33
41	Ab initio and semiempirical cluster studies on the reactivity of the vanadium pentoxide (010) surface. Journal of Electron Spectroscopy and Related Phenomena, 1994, 69, 89-98.	0.8	44
42	Adsorption of toluene on vanadium pentoxide surfaces. Quantum chemical study. Journal of Molecular Catalysis, 1993, 82, 457-466.	1.2	20
43	Oxidation of hydrocarbons on transition metal oxide catalysts â€" quantum chemical studies. Journal of Molecular Catalysis, 1991, 70, 277-333.	1.2	48
44	Ab initioMRD CI calculations for ground and excited states of Cu2molecule. Molecular Physics, 1982, 47, 945-957.	0.8	21