

# MaÅ,gorzata Witko

## List of Publications by Year in descending order

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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	Nitrite binding to metmyoglobin and methemoglobin in comparison to nitric oxide binding. Journal of Biological Inorganic Chemistry, 2002, 7, 165-176.	1.1	49
2	Oxidation of hydrocarbons on transition metal oxide catalysts – quantum chemical studies. Journal of Molecular Catalysis, 1991, 70, 277-333.	1.2	48
3	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
4	Reactions of the $[\text{Fe}(\text{CN})_5\text{NO}]^{2-}$ complex with biologically relevant thiols. New Journal of Chemistry, 2002, 26, 1495-1502.	1.4	42
5	Oxygen vacancy formation on clean and hydroxylated low-index $\text{V}_2\text{O}_5$ surfaces: A density functional investigation. Physical Review B, 2009, 79, .	1.1	39
6	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
7	Reduction and re-oxidation of molybdena and vanadia: DFT cluster model studies. Catalysis Today, 2005, 99, 241-253.	2.2	36
8	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
9	Quantum-chemical description of the active sites for the selective oxidation of hydrocarbons. Catalysis Today, 1996, 32, 89-95.	2.2	33
10	Electronic structure of $\text{MoO}_2$ . DFT periodic and cluster model studies. Applied Catalysis A: General, 2011, 391, 137-143.	2.2	30
11	Surface oxygen in catalysts based on transition metal oxides. Catalysis Today, 2004, 91-92, 171-176.	2.2	29
12	Polyhydroxyalkanoate-derived hydrogen-bond donors for the synthesis of new deep eutectic solvents. Green Chemistry, 2019, 21, 3116-3126.	4.6	29
13	Structural, topographical, and mechanical characteristics of purified polyhydroxyoctanoate polymer. Journal of Applied Polymer Science, 2019, 136, 47192.	1.3	28
14	Relative stability of low-index $\text{V}_2\text{O}_5$ surfaces: a density functional investigation. Journal of Physics Condensed Matter, 2009, 21, 095008.	0.7	27
15	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
16	How to select an optimal neural model of chemical reactivity?. Neurocomputing, 2008, 72, 241-256.	3.5	23
17	Following nature – Theoretical studies on factors modulating catalytic activity of porphyrins. Journal of Molecular Catalysis A, 2006, 258, 376-380.	4.8	22
18	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

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19	Ab initio MRD CI calculations for ground and excited states of Cu <sub>2</sub> molecule. <i>Molecular Physics</i> , 1982, 47, 945-957.	0.8	21
20	Ligation of water to magnesium chelates of biological importance. <i>Journal of Molecular Modeling</i> , 2013, 19, 4661-4667.	0.8	21
21	Adsorption of toluene on vanadium pentoxide surfaces. Quantum chemical study. <i>Journal of Molecular Catalysis</i> , 1993, 82, 457-466.	1.2	20
22	Novel bioresorbable tricalcium phosphate/polyhydroxyoctanoate (TCP/PHO) composites as scaffolds for bone tissue engineering applications. <i>Journal of the Mechanical Behavior of Biomedical Materials</i> , 2019, 98, 235-245.	1.5	20
23	Influence of Anatase Support on Geometrical Structure of Vanadium Oxide at Varying Temperatures and Pressures. Periodic DFT Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 4216-4225.	1.5	18
24	Application of the DFT Theory to Study Cobalamin Complexes. <i>Structural Chemistry</i> , 2004, 15, 431-435.	1.0	17
25	Mechanistic Insight into Peroxo Shunt Formation of Biomimetic Models for Compound II, Their Reactivity toward Organic Substrates, and the Influence of N-Methylimidazole Axial Ligation. <i>Chemistry - A European Journal</i> , 2014, 20, 2328-2343.	1.7	17
26	Sixth International Symposium. <i>Applied Surface Science</i> , 2007, 253, 5565-5569.	3.1	14
27	Allylic oxidation of cyclohexene catalyzed by manganese porphyrins: DFT studies. <i>Catalysis Today</i> , 2011, 169, 10-15.	2.2	14
28	Functionalized tricalcium phosphate and poly(3-hydroxyoctanoate) derived composite scaffolds as platforms for the controlled release of diclofenac. <i>Ceramics International</i> , 2021, 47, 3876-3883.	2.3	13
29	From activation of dioxygen to formation of high-valent oxo species: Ab initio DFT studies. <i>Journal of Molecular Catalysis A</i> , 2007, 275, 113-120.	4.8	12
30	The reaction mechanism of chiral hydroxylation of <i>p</i> -OH and <i>p</i> -NH <sub>2</sub> substituted compounds by ethylbenzene dehydrogenase. <i>Canadian Journal of Chemistry</i> , 2013, 91, 775-786.	0.6	12
31	Ammonium adsorption on Brønsted acidic centers on low-index vanadium pentoxide surfaces. <i>Journal of Molecular Modeling</i> , 2013, 19, 4487-4501.	0.8	12
32	Theoretical density functional theory studies on interactions of small biologically active molecules with isolated heme group. <i>Journal of Computational Chemistry</i> , 2007, 28, 825-831.	1.5	11
33	Physicochemical and Biological Characterisation of Diclofenac Oligomeric Poly(3-hydroxyoctanoate) Hybrids as <sup>125</sup> I-TCP Ceramics Modifiers for Bone Tissue Regeneration. <i>International Journal of Molecular Sciences</i> , 2020, 21, 9452.	1.8	11
34	Factors controlling the reactivity of divalent metal ions towards pheophytin a. <i>Journal of Biological Inorganic Chemistry</i> , 2017, 22, 941-952.	1.1	9
35	Oxygen Sites at Molybdena and Vanadia Surfaces: Energetics of the Re-Oxidation Process. <i>Collection of Czechoslovak Chemical Communications</i> , 2004, 69, 121-140.	1.0	9
36	Chemical nature of point defects at the (VO) <sub>2</sub> P <sub>2</sub> O <sub>7</sub> (100) surface. <i>Surface Science</i> , 2003, 538, 160-170.	0.8	8

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37	Metallobacteriochlorophylls as potential dual agents for photodynamic therapy and chemotherapy. <i>Journal of Molecular Modeling</i> , 2013, 19, 4155-4161.	0.8	7
38	Surface Cluster Models for V <sub>2</sub> O <sub>5</sub> - Studies of the Importance of Local Geometry. <i>Collection of Czechoslovak Chemical Communications</i> , 1998, 63, 1355-1367.	1.0	5
39	Ligand binding properties of cobalamins. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 411-419.	0.5	5
40	Hydrogen peroxide as oxidant in bio-mimetic catalysis by manganese porphyrin: Theoretical DFT studies. <i>Canadian Journal of Chemistry</i> , 2013, 91, 642-647.	0.6	5
41	The Influence of Structural Parameters on the Reactivity of Model Complexes for Compound II: A Mini Review. <i>Topics in Catalysis</i> , 2014, 57, 946-952.	1.3	4
42	Comparison of Catalytic Properties of Vanadium Centers Introduced into BEA Zeolite and Present on (010) V <sub>2</sub> O <sub>5</sub> Surface – DFT Studies. <i>Catalysts</i> , 2020, 10, 1080.	1.6	3
43	Tungsten and Molybdenum Heteropolyanions with Different Central Ions – Correlation between Theory and Experiment. <i>Molecules</i> , 2022, 27, 187.	1.7	2
44	Nanospace constraints in mesoporous silica carriers – A factor of critical importance in promoting the catalytic activity of supported ruthenium (II) complex with hemilabile phosphine ligand. <i>Applied Catalysis A: General</i> , 2012, 427-428, 16-23.	2.2	1