

Renata Tokarz-Sobieraj

List of Publications by Year in descending order

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36
papers

1,122
citations

331670

21
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377865

34
g-index

37
all docs

37
docs citations

37
times ranked

1293
citing authors

#	ARTICLE	IF	CITATIONS
1	Vanadium pentoxide I. Structures and properties. Applied Catalysis A: General, 1997, 157, 3-22.	4.3	190
2	Properties of oxygen sites at the MoO ₃ (010) surface: density functional theory cluster studies and photoemission experiments. Surface Science, 2001, 489, 107-125.	1.9	166
3	Adsorption and reactions at the (010) V ₂ O ₅ surface: cluster model studies. Catalysis Today, 1999, 50, 553-565.	4.4	72
4	Oxygen vacancies at oxide surfaces: ab initio density functional theory studies on vanadium pentoxide. Applied Physics A: Materials Science and Processing, 2001, 72, 429-442.	2.3	54
5	Quantum chemical calculations of molecular properties of V ₂ O ₅ clusters. Journal of Molecular Catalysis, 1991, 66, 205-214.	1.2	44
6	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.	1.7	44
7	Vanadium pentoxide. II. Quantum chemical modeling. Applied Catalysis A: General, 1997, 157, 23-44.	4.3	40
8	Humidity induced deactivation of Al ₂ O ₃ and SiO ₂ supported Pd, Pt, Pd-Pt catalysts in H ₂ +O ₂ recombination reaction: The catalytic, microcalorimetric and DFT studies. Applied Catalysis A: General, 2015, 501, 27-40.	4.3	39
9	Hydrogen assisted oxygen desorption from the V ₂ O ₅ (010) surface. Topics in Catalysis, 2000, 11/12, 67-75.	2.8	36
10	Reduction and re-oxidation of molybdena and vanadia: DFT cluster model studies. Catalysis Today, 2005, 99, 241-253.	4.4	36
11	Dependence of metathesis activity of Mo-methylidene sites on their location on (100) γ -Al ₂ O ₃ theoretical study. Catalysis Today, 2005, 101, 163-173.	4.4	33
12	Electronic structure of vanadyl pyrophosphate: cluster model studies. Journal of Molecular Catalysis A, 2001, 166, 59-72.	4.8	31
13	Electronic structure of MoO ₂ . DFT periodic and cluster model studies. Applied Catalysis A: General, 2011, 391, 137-143.	4.3	30
14	Surface oxygen in catalysts based on transition metal oxides. Catalysis Today, 2004, 91-92, 171-176.	4.4	29
15	Electronic properties of the VO ₂ (011) surface: density functional cluster calculations. Surface Science, 2001, 491, 77-87.	1.9	27
16	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.	4.3	26
17	Charge sensitivity analysis of oxide catalysts: V ₂ O ₅ clusters and (n-V ₂ O ₅) ⁻ H(in ₂) systems. Journal of Molecular Catalysis, 1992, 77, 165-180.	1.2	24
18	The role of atoms which terminate clusters: Quantum chemical study. Journal of Molecular Catalysis, 1991, 66, 357-366.	1.2	23

#	ARTICLE	IF	CITATIONS
19	A role of Au-content in performance of Pd-Au/SiO ₂ and Pd-Au/Al ₂ O ₃ catalyst in the hydrogen and oxygen recombination reaction. The microcalorimetric and DFT studies. Applied Catalysis A: General, 2016, 517, 196-210.	4.3	23
20	Heterogeneity of V ₂ O ₅ (010) surfaces – the role of alkali metal dopants. Topics in Catalysis, 2006, 38, 105-115.	2.8	22
21	Quantum Chemical Description of Oxygen Activation Process on Co, Mn, and Mo Porphyrins. Journal of Chemical Theory and Computation, 2007, 3, 914-920.	5.3	22
22	Adsorption of toluene on vanadium pentoxide surfaces. Quantum chemical study. Journal of Molecular Catalysis, 1993, 82, 457-466.	1.2	20
23	Hydroxylation of phenol by hydrogen peroxide catalyzed by heteropoly compounds in presence of glycerol as green solvent. Catalysis Today, 2015, 257, 80-85.	4.4	15
24	Interaction of oxygen with the surface of vanadia catalysts. Journal of Molecular Catalysis A, 2007, 277, 27-34.	4.8	14
25	Theoretical study of 1-(4-hexylcyclohexyl)-4-isothiocyanatobenzene: molecular properties and spectral characteristics. Journal of Molecular Modeling, 2009, 15, 935-943.	1.8	12
26	Generation of acidic sites in Al, Ga, In salts of molybdenum and tungsten Keggin-type heteropolyacids. DFT modeling and catalytic tests. Catalysis Today, 2015, 257, 72-79.	4.4	12
27	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
28	DFT investigation of molybdenum (oxo)carbide formation from MoO ₃ . Structural Chemistry, 2012, 23, 1417-1424.	2.0	8
29	Surface Cluster Models for V ₂ O ₅ - Studies of the Importance of Local Geometry. Collection of Czechoslovak Chemical Communications, 1998, 63, 1355-1367.	1.0	5
30	Electronic Properties of the Active Sites Present at the (011) Surface of MoO ₂ . Adsorption Science and Technology, 2007, 25, 583-596.	3.2	5
31	Cu ²⁺ in Keggin anion – Influence of copper position on electronic structure/redox properties of heteropolyacids. DFT cluster model study. Journal of Molecular Structure, 2017, 1135, 20-25.	3.6	3
32	Comparison of Catalytic Properties of Vanadium Centers Introduced into BEA Zeolite and Present on (010) V ₂ O ₅ Surface – DFT Studies. Catalysts, 2020, 10, 1080.	3.5	3
33	Tungsten and Molybdenum Heteropolyanions with Different Central Ions – Correlation between Theory and Experiment. Molecules, 2022, 27, 187.	3.8	2
34	Quantum Modeling of Geometric Electronic Structures of Some Mesogenic Systems. Molecular Crystals and Liquid Crystals, 2008, 480, 219-228.	0.9	1
35	Oxygen Adsorption and Activation on Cobalt Center in Modified Keggin Anion-DFT Calculations. Catalysts, 2020, 10, 144.	3.5	1
36	Quantum chemical DFT calculations of electronic and geometric structure of 4-(2-hexyloxy-ethoxy)-4'-cyano biphenyl (6O2OCB), 2004, , .		0