Renata Tokarz-Sobieraj

List of Publications by Year
in descending order

36 papers	1,122 citations	331670 21 h-index	377865 34 g-index
37 all docs	37 docs citations	37 times ranked	1293 citing authors

#	Article	IF	Citations
1	Tungsten and Molybdenum Heteropolyanions with Different Central Ionsâ€"Correlation between Theory and Experiment. Molecules, 2022, 27, 187.	3.8	2
2	Comparison of Catalytic Properties of Vanadium Centers Introduced into BEA Zeolite and Present on (010) V2O5 Surfaceâ€"DFT Studies. Catalysts, 2020, 10, 1080.	3.5	3
3	Oxygen Adsorption and Activation on Cobalt Center in Modified Keggin Anion-DFT Calculations. Catalysts, 2020, 10, 144.	3.5	1
4	Cu2+ in Keggin anion â€" 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
5	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
6	A role of Au-content in performance of Pd-Au/SiO2 and Pd-Au/Al2O3 catalyst in the hydrogen and oxygen recombination reaction. The microcalorimetric and DFT studies. Applied Catalysis A: General, 2016, 517, 196-210.	4.3	23
7	Humidity induced deactivation of Al2O3 and SiO2 supported Pd, Pt, Pd-Pt catalysts in H2+O2 recombination reaction: The catalytic, microcalorimetric and DFT studies. Applied Catalysis A: General, 2015, 501, 27-40.	4.3	39
8	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
9	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
10	DFT investigation of molybdenum (oxo)carbide formation from MoO3. Structural Chemistry, 2012, 23, 1417-1424.	2.0	8
11	Electronic structure of MoO2. DFT periodic and cluster model studies. Applied Catalysis A: General, 2011, 391, 137-143.	4.3	30
12	Theoretical study of 1-(4-hexylcyclohexyl)-4-isothiocyanatobenzene: molecular properties and spectral characteristics. Journal of Molecular Modeling, 2009, 15, 935-943.	1.8	12
13	Quantum Modeling of Geometric Electronic Structures of Some Mesogenic Systems. Molecular Crystals and Liquid Crystals, 2008, 480, 219-228.	0.9	1
14	Electronic Properties of the Active Sites Present at the (011) Surface of MoO₂. Adsorption Science and Technology, 2007, 25, 583-596.	3.2	5
15	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
16	Interaction of oxygen with the surface of vanadia catalysts. Journal of Molecular Catalysis A, 2007, 277, 27-34.	4.8	14
17	Heterogeneity of V2O5(010) surfaces â€" the role of alkali metal dopants. Topics in Catalysis, 2006, 38, 105-115.	2.8	22
18	Reduction and re-oxidation of molybdena and vanadia: DFT cluster model studies. Catalysis Today, 2005, 99, 241-253.	4.4	36

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19	Dependence of metathesis activity of Mo-methylidene sites on their location on (100) Î³-Al2O3â€"a theoretical study. Catalysis Today, 2005, 101, 163-173.	4.4	33
20	Surface oxygen in catalysts based on transition metal oxides. Catalysis Today, 2004, 91-92, 171-176.	4.4	29
21	‹title›Quantum chemical DFT calculations of electronic and geometric structure of 4-(2-hexyloxy-ethoxy)-4`-cyano biphenyl (6O2OCB)‹/title›. , 2004, , .		0
22	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
23	Properties of oxygen sites at the MoO3(010) surface: density functional theory cluster studies and photoemission experiments. Surface Science, 2001, 489, 107-125.	1.9	166
24	Electronic properties of the VO2(011) surface: density functional cluster calculations. Surface Science, 2001, 491, 77-87.	1.9	27
25	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
26	Electronic structure of vanadyl pyrophosphate: cluster model studies. Journal of Molecular Catalysis A, 2001, 166, 59-72.	4.8	31
27	Hydrogen assisted oxygen desorption from the V2O5(010) surface. Topics in Catalysis, 2000, 11/12, 67-75.	2.8	36
28	Adsorption and reactions at the (010) V2O5 surface: cluster model studies. Catalysis Today, 1999, 50, 553-565.	4.4	72
29	Surface Cluster Models for V2O5 - Studies of the Importance of Local Geometry. Collection of Czechoslovak Chemical Communications, 1998, 63, 1355-1367.	1.0	5
30	Vanadium pentoxide I. Structures and properties. Applied Catalysis A: General, 1997, 157, 3-22.	4.3	190
31	Vanadium pentoxide. II. Quantum chemical modeling. Applied Catalysis A: General, 1997, 157, 23-44.	4.3	40
32	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
33	Adsorption of toluene on vanadium pentoxide surfaces. Quantum chemical study. Journal of Molecular Catalysis, 1993, 82, 457-466.	1.2	20
34	Charge sensitivity analysis of oxide catalysts: V2O5 clusters and (n-V2O5)î—¸H(in2) systems. Journal of Molecular Catalysis, 1992, 77, 165-180.	1.2	24
35	Quantum chemical calculations of molecular properties of V2O5 clusters. Journal of Molecular Catalysis, 1991, 66, 205-214.	1.2	44
36	The role of atoms which terminate clusters: Quantum chemical study. Journal of Molecular Catalysis, 1991, 66, 357-366.	1.2	23