

# Parasuraman Selvam

## List of Publications by Year in descending order

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211  
papers

5,646  
citations

81743

39  
h-index

106150

65  
g-index

220  
all docs

220  
docs citations

220  
times ranked

5493  
citing authors

#	ARTICLE	IF	CITATIONS
1	Ordered Mesoporous Carbon-supported Morphologically-controlled Nano-Gold: Role of Support as well as the Shape and Size of Gold Nanoparticles on the Selective Oxidation of Glycerol. ChemCatChem, 2022, 14, .	1.8	1
2	Hydrodeoxygenation kinetics of syringol, guaiacol and phenol over H-ZSM-5. Catalysis Communications, 2021, 148, 106164.	1.6	27
3	Water-Driven Structural Transformation in Cobalt Trimesate Metal-Organic Frameworks. Energies, 2021, 14, 4751.	1.6	8
4	Hydrodeoxygenation of Bio-Oil from Fast Pyrolysis of Pinewood Over Various Catalysts. Springer Proceedings in Energy, 2021, , 141-148.	0.2	0
5	Surfactant-mediated and Morphology-controlled Nanostructured LiFePO <sub>4</sub> /Carbon Composite as a Promising Cathode Material for Li-ion Batteries. ChemistryOpen, 2020, 9, 23-31.	0.9	8
6	Production of xylooligosaccharides from xylan catalyzed by endo-1,4-β-D-xylanase-immobilized nanoscale carbon, silica and zirconia matrices. Molecular Catalysis, 2020, 484, 110745.	1.0	7
7	Evaluation of visible-light driven photocatalytic reaction by porphyrin coupled TiO <sub>2</sub> nanotubes obtained via rapid breakdown anodization. Journal of Environmental Chemical Engineering, 2020, 8, 104382.	3.3	15
8	Nanostructured zeolite with brain-coral morphology and tailored acidity: a self-organized hierarchical porous material with MFI topology. CrystEngComm, 2020, 22, 6275-6286.	1.3	3
9	Electrochemical performance of nano-sized LiFePO <sub>4</sub> -embedded 3D-cubic ordered mesoporous carbon and nitrogenous carbon composites. RSC Advances, 2020, 10, 30406-30414.	1.7	5
10	Periodic mesoporous titania with anatase and bronze phases – the new generation photocatalyst: synthesis, characterisation, and application in environmental remediation. New Journal of Chemistry, 2020, 44, 16269-16284.	1.4	5
11	Adsorption of hydrogen and carbon dioxide in zeolitic imidazolate framework structure with SOD topology: experimental and modelling studies. Adsorption, 2020, 26, 1027-1038.	1.4	21
12	Immobilization of Recombinant Endo-1,4-β-D-xylanase on Ordered Mesoporous Matrices for Xylooligosaccharides Production. ChemistrySelect, 2019, 4, 11214-11221.	0.7	8
13	Nanoarchitected peroxidase-mimetic nanozymes: mesoporous nanocrystalline Fe <sup>2+</sup> - or Fe <sup>3+</sup> -iron oxide?. Journal of Materials Chemistry B, 2019, 7, 5412-5422.	2.9	72
14	Electrochemical performance of nano-LiFePO <sub>4</sub> embedded ordered mesoporous nitrogenous carbon composite as cathode material for Li-ion battery applications. Journal of Electroanalytical Chemistry, 2019, 848, 113242.	1.9	19
15	The Enhanced Catalytic Performance and Stability of Ordered Mesoporous Carbon Supported Nano-Gold with High Structural Integrity for Glycerol Oxidation. Chemical Record, 2019, 19, 1913-1925.	2.9	20
16	Novel ionic liquid-templated ordered mesoporous aluminosilicates: Synthesis, characterization and catalytic properties. Microporous and Mesoporous Materials, 2019, 275, 172-179.	2.2	12
17	Synthesis and characterization of Keggin-type polyoxometalate/zirconia nanocomposites – Comparison of its photocatalytic activity towards various organic pollutants. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 370, 26-40.	2.0	42
18	Hydrogenolysis of glycerol over silica-supported copper-nanocatalyst: Effect of precipitating-agent and copper metal-loading. Molecular Catalysis, 2018, 458, 307-316.	1.0	18

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19	Selective production of aromatic hydrocarbons from lignocellulosic biomass via catalytic fast-hydrolysis using W2C/Al <sub>2</sub> O <sub>3</sub> . Catalysis Communications, 2018, 110, 68-73.	1.6	32
20	Ordered mesoporous nanocrystalline titania: A promising new class of photocatalytic materials. Catalysis Today, 2018, 309, 202-211.	2.2	18
21	Fabrication of SPAEK-cerium zirconium oxide nanotube composite membrane with outstanding performance and durability for vanadium redox flow batteries. Journal of Materials Chemistry A, 2018, 6, 20205-20213.	5.2	44
22	Sulfonic Acid Functionalized Ordered Mesoporous Silica and their Application as Highly Efficient and Selective Heterogeneous Catalysts in the Formation of 1,2-Monoacetone-D-glucose. ChemCatChem, 2018, 10, 5610-5618.	1.8	12
23	Rational design, synthesis, characterization and catalytic properties of high-quality low-silica hierarchical FAU- and LTA-type zeolites. Scientific Reports, 2018, 8, 16291.	1.6	22
24	Hydrogen Sorption Characteristics of Ordered Mesoporous Carbons: Experimental and Modeling View Point. Journal of Chemical & Engineering Data, 2018, , .	1.0	4
25	A Remarkable Catalytic Activity of Hierarchical Zeolite (Zr-5) for Tertiary Butylation of Phenol with Enhanced 2,4-Di- <i>t</i> -Butylphenol Selectivity. ChemCatChem, 2018, 10, 3978-3984.	1.8	10
26	Theory as a driving force to understand reactions on nanoparticles: general discussion. Faraday Discussions, 2018, 208, 147-185.	1.6	3
27	Application of new nanoparticle structures as catalysts: general discussion. Faraday Discussions, 2018, 208, 575-593.	1.6	1
28	Control of catalytic nanoparticle synthesis: general discussion. Faraday Discussions, 2018, 208, 471-495.	1.6	3
29	ORDERED NANOSTRUCTURED CARBONS, NCCR-41 AND CMK-3: SYNTHESIS, CHARACTERIZATION, AND HYDROGEN SORPTION STUDIES. Catalysis in Green Chemistry and Engineering, 2018, 1, 235-246.	0.2	3
30	Ordered Mesoporous Silica-Based Precious Metal Catalysts for NO Reduction. Advanced Porous Materials, 2018, 6, 73-79.	0.3	0
31	Acid-Mediated Synthesis of Ordered Mesoporous Aluminosilicates: The Challenge and the Promise. Chemistry - A European Journal, 2017, 23, 1604-1612.	1.7	16
32	Designing ordered mesoporous aluminosilicates under acidic conditions via an intrinsic hydrolysis method. Dalton Transactions, 2017, 46, 770-779.	1.6	12
33	Preparation and characterization of CNSR functionalized Fe <sub>3</sub> O <sub>4</sub> magnetic nanoparticles: An efficient adsorbent for the removal of cadmium ion from water. Journal of Environmental Chemical Engineering, 2017, 5, 4539-4546.	3.3	44
34	A visible-light active catechol-metal oxide carbonaceous polymeric material for enhanced photocatalytic activity. Journal of Materials Chemistry A, 2017, 5, 384-396.	5.2	68
35	Synthesis of $\gamma$ -alumina nanoparticles by wire-explosion process: Characterisation and formation mechanism. , 2017, , .		2
36	Biological Evolution of New Intercalated Layered Double Hydroxides: Anticancer, Antibacterial and Photocatalytic Studies. ChemistrySelect, 2017, 2, 11717-11726.	0.7	4

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37	Li-ion kinetics in LiFePO <sub>4</sub> /carbon nanocomposite prepared by a two-step process: The role of phase composition. <i>Electrochimica Acta</i> , 2016, 209, 565-573.	2.6	19
38	An efficient mesoporous carbon nitride (g-C <sub>3</sub> N <sub>4</sub> ) functionalized Pd catalyst for carbon-carbon bond formation reactions. <i>RSC Advances</i> , 2016, 6, 49376-49386.	1.7	35
39	Mesoporous Iron Oxide Nanoparticles for Magnetically Triggered Release of Doxorubicin and Hyperthermia Treatment. <i>Chemistry - A European Journal</i> , 2016, 22, 17020-17028.	1.7	39
40	Designing new catalysts: synthesis of new active structures: general discussion. <i>Faraday Discussions</i> , 2016, 188, 131-159.	1.6	4
41	Effect of the Titanium Nanoparticle on the Quantum Chemical Characterization of the Liquid Sodium Nanofluid. <i>Journal of Physical Chemistry B</i> , 2016, 120, 3527-3539.	1.2	0
42	Ionic Liquid Templated Synthesis of Hexagonal (IITM-41) and Cubic (IITM-48) Ordered Mesoporous Silicates. <i>Advanced Porous Materials</i> , 2016, 4, 24-30.	0.3	6
43	Amino-Functionalized Phosphotungstic Acid-Anchored Mesoporous Molecular Sieves: Highly Efficient Catalysts for Selective Epoxidation of Cyclohexene. <i>Advanced Porous Materials</i> , 2016, 4, 110-117.	0.3	4
44	Investigation of Nano-Molybdenum Carbide Particle Produced by Wire-Explosion Process. <i>IEEE Transactions on Plasma Science</i> , 2015, 43, 3470-3475.	0.6	10
45	Crystal structure of aquadioxido(2-[[[2-oxidoethyl]imino]methyl]phenolato- $\lambda^3$ )-molybdenum(V). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015, 71, m35-m36.		1
46	Crystal structure of (2-formylphenolato- $\lambda^2$ )-oxido(2-[[[2-oxidoethyl]imino]methyl]phenolato- $\lambda^3$ )-vanadium(V). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015, 71, m104-m105.	0.2	0
47	Ordered mesoporous carbon-supported nano-platinum catalysts: application in direct methanol fuel cells. <i>Sustainable Energy Developments</i> , 2015, , 131-157.	0.3	1
48	Development of the bifunctional catalyst Mn-Fe-Beta for selective catalytic reduction of nitrogen oxides. <i>Russian Chemical Bulletin</i> , 2014, 63, 389-395.	0.4	11
49	Crystal structure of bis(acetato- $\lambda^2$ )-diaqua(2,2'-bipyridine- $\lambda^2$ )-manganese(II). <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014, 70, m326-m327.	0.2	2
50	Combined NO <sub>x</sub> Selective Catalytic Reduction and NH <sub>3</sub> -slip Oxidation Activity of Composite [Fe-Beta + Fe(Mn)MCM-48] Catalysts. <i>Mendelevov Communications</i> , 2014, 24, 313-315.	0.6	6
51	Fast and Standard Selective Catalytic Reduction in NH <sub>3</sub> -DeNO <sub>x</sub> : Pathways Discrimination as a Key Step for the Understanding of Kinetics. <i>Mendelevov Communications</i> , 2014, 24, 311-312.	0.6	6
52	Synthesis, characterization and electrocatalytic properties of nano-platinum-supported mesoporous carbon molecular sieves, Pt/NCCR-41. <i>Catalysis Today</i> , 2012, 198, 85-91.	2.2	16
53	Platinum-supported mesoporous carbon (Pt/CMK-3) as anodic catalyst for direct methanol fuel cell applications: The effect of preparation and deposition methods. <i>Progress in Natural Science: Materials International</i> , 2012, 22, 616-623.	1.8	52
54	Selective Oxidation of Alkenes over Uranyl-Anchored Mesoporous MCM-41 Molecular Sieves. <i>Journal of Physical Chemistry C</i> , 2011, 115, 1922-1931.	1.5	16

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55	Specific role of polymorphs of supporting titania in catalytic CO oxidation on gold. <i>Catalysis Today</i> , 2011, 164, 325-331.	2.2	10
56	Platinum group metals substituted MCM-41 molecular sieves: Synthesis, characterization and application as novel catalysts for the reduction of NO by CO. <i>Journal of Molecular Catalysis A</i> , 2009, 314, 49-54.	4.8	15
57	Probing the Fe(III) sites in mesoporous FeMCM-41. <i>Catalysis Today</i> , 2009, 141, 103-108.	2.2	5
58	Hydrogenation of nitrobenzene over palladium-supported catalysts—Effect of support. <i>Applied Catalysis A: General</i> , 2009, 353, 160-165.	2.2	132
59	Removal of rhodamine B from aqueous solution by adsorption onto sodium montmorillonite. <i>Journal of Hazardous Materials</i> , 2008, 155, 39-44.	6.5	212
60	Supported 12-tungstophosphoric acid: An efficient and selective solid acid catalyst for tert-butylation of phenol and cresols. <i>Catalysis Communications</i> , 2008, 9, 1545-1550.	1.6	30
61	Uranyl-Anchored MCM-41 as a Highly Efficient Photocatalyst in the Oxidative Destruction of Short Chain Linear Alkanes: An in situ FTIR Study. <i>Journal of Physical Chemistry C</i> , 2008, 112, 15832-15843.	1.5	14
62	Theoretical Simulation of Dielectric Breakdown by Molecular Dynamics and Tight-Binding Quantum Chemistry Methods. <i>Japanese Journal of Applied Physics</i> , 2007, 46, 1853-1858.	0.8	6
63	Large-Scale Electronic Structure Calculation on Blue Phosphor BaMgAl10O17:Eu2+ Using Tight-Binding Quantum Chemistry Method Implemented for Rare-Earth Elements. <i>Japanese Journal of Applied Physics</i> , 2007, 46, 2534-2541.	0.8	12
64	Theoretical Investigation on Electrical and Electronic Properties of Carbon Materials. <i>Japanese Journal of Applied Physics</i> , 2007, 46, 2650-2654.	0.8	5
65	Novel computational chemistry approaches for studying physico-chemical properties of zeolite materials. <i>Microporous and Mesoporous Materials</i> , 2007, 101, 324-333.	2.2	7
66	Fresh and calcined supported 12-tungstosilicic acid: Synthesis, characterization and application to some acid catalyzed reactions. <i>Journal of Molecular Catalysis A</i> , 2007, 275, 14-24.	4.8	13
67	An in situ FT-IR study of photo-oxidation of alcohols over uranyl-anchored MCM-41: Possible reaction pathways. <i>Journal of Catalysis</i> , 2007, 247, 1-19.	3.1	22
68	A highly selective, heterogeneous route to enones from allylic and benzylic compounds over mesoporous CrMCM-41 molecular sieves. <i>Journal of Catalysis</i> , 2007, 249, 394-396.	3.1	40
69	Structured TiO <sub>2</sub> based catalysts for clean water technologies. <i>Studies in Surface Science and Catalysis</i> , 2006, 162, 151-158.	1.5	7
70	H-MOR: Density functional investigation for the relative strength of Brønsted acid sites and dynamics simulation of NH <sub>3</sub> protonation—deprotonation. <i>Journal of Molecular Catalysis A</i> , 2006, 243, 1-7.	4.8	16
71	Thermally stable trivalent iron-substituted hexagonal mesoporous aluminophosphate (FeHMA) molecular sieves: Synthesis, characterization, and catalytic properties. <i>Journal of Catalysis</i> , 2006, 238, 88-99.	3.1	38
72	Heterogeneous Photocatalytic Degradation of Methanol over Uranyl-Anchored Nanoporous MCM-41 and MCM-48. <i>Journal of Nanoscience and Nanotechnology</i> , 2006, 6, 1811-1814.	0.9	2

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73	Transition-Metal (Ti,V,Cr,Mn,Fe,Co,Cu) Containing Ordered Nanoporous Materials:Novel Heterogeneous Catalysts for Selective Oxidation Reactions. Journal of Nanoscience and Nanotechnology, 2006, 6, 1758-1764.	0.9	3
74	Regio- and Chemoselective Reduction of Aromatic Nitro and Carbonyl Compounds Over Novel Bakers Yeast Immobilized Nanoporous Silicates. Letters in Organic Chemistry, 2006, 3, 901-904.	0.2	4
75	COMPUTATIONAL CHEMISTRY FOR INDUSTRIAL INNOVATION. Reviews in Chemical Engineering, 2006, 22, .	2.3	18
76	Theoretical Investigation of Electrical and Electronic Properties of Carbon Materials. , 2006, , .		0
77	Theoretical Simulation of Dielectric Breakdown by Molecular Dynamics and Tight-Binding Quantum Chemistry Methods. , 2006, , .		0
78	Theoretical Study on the Electronic and Structural Properties of p-Type Transparent Conducting Metal Oxides. , 2006, , .		0
79	Development of New Calculation Method for Rare Earth Element and Large Scale Electronic Structure Calculation of Blue Phosphor BaMgAl10O17:Eu2+. , 2006, , .		0
80	Vapor-phase photocatalytic oxidation of volatile organic compounds over novel uranyl-anchored MCM-41 heterogeneous catalyst. Studies in Surface Science and Catalysis, 2005, , 787-794.	1.5	1
81	Synthesis and characterization of new photoresponsive acrylamide polymers having pendant chalcone moieties. Reactive and Functional Polymers, 2005, 62, 179-193.	2.0	23
82	Transition metal (Cu, Cr, and V) modified MCM-41 for the catalytic wet air oxidation of aniline. Microporous and Mesoporous Materials, 2005, 86, 287-294.	2.2	87
83	Tight-binding quantum chemical molecular dynamics method: a novel approach to the understanding and design of new materials and catalysts. Catalysis Today, 2005, 100, 11-25.	2.2	16
84	Synthesis, characterization and photocrosslinking properties of polyacrylamides having bromo substituted pendant cinnamoyl moieties. European Polymer Journal, 2005, 41, 35-45.	2.6	6
85	Studies on photocrosslinkable copolymers of 4-methacryloyloxyphenyl-3,4-dimethoxystyryl ketone and methyl methacrylate. European Polymer Journal, 2005, 41, 831-841.	2.6	14
86	The effect of vanadium sources on the synthesis and catalytic activity of VMCM-41. Journal of Catalysis, 2005, 229, 64-71.	3.1	51
87	Synthesis and characterization of divalent cobalt-substituted mesoporous aluminophosphate molecular sieves and their application as novel heterogeneous catalysts for the oxidation of cycloalkanes. Journal of Catalysis, 2005, 233, 276-287.	3.1	46
88	Tight-Binding Quantum Chemical Molecular Dynamics Method: a Novel Approach to the Understanding and Design of New Materials and Catalysts. ChemInform, 2005, 36, no.	0.1	0
89	Magnetization Studies of Mercury-Cuprates and Its Precursors. Journal of Superconductivity and Novel Magnetism, 2005, 18, 475-480.	0.5	1
90	1-(4-Chlorophenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o405-o407.	0.2	4

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91	3-(3-Hydroxyphenyl)-1-(4-methoxyphenyl)prop-2-en-1-one. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o743-o745.	0.2	3
92	Chemical reaction dynamics of PeCB and TCDD decomposition: A tight-binding quantum chemical molecular dynamics study with first-principles parameterization. International Journal of Quantum Chemistry, 2005, 102, 318-327.	1.0	21
93	Synthesis protocol and superconducting properties of (Hg,Cr)Sr <sub>2</sub> CuO <sub>4</sub> + $\hat{\Gamma}$ . Superconductor Science and Technology, 2005, 18, 264-270.	1.8	0
94	Synthesis, structural parameters and superconducting properties of 1201-type (Hg,M)Sr <sub>2</sub> CuO <sub>4</sub> + $\hat{\Gamma}$ (M = Tl, Bi, Pb, Hg, Sr). Physica C: Superconductivity, 2005, 423-424, 1-5.	1.8	5
95	Copolymers of 4-(4-(2,4-dimethoxycinnamoyl)phenyl)Acrylate and MMA: Synthesis, Characterization, Photocrosslinking Properties, and Monomer Reactivity Ratios. Journal of Macromolecular Science - Pure and Applied Chemistry, 2004, 41, 791-809.	1.2	3
96	IMPACT OF PRECURSOR SOURCE ON THE STRUCTURAL AND SUPERCONDUCTING PROPERTIES OF (Hg,Cr)Sr <sub>2</sub> CuO <sub>4</sub> + $\hat{\Gamma}$ . Modern Physics Letters B, 2004, 18, 1517-1524.	1.0	1
97	Combinatorial computational chemistry approach to the design of metal catalysts for deNO <sub>x</sub> . Applied Surface Science, 2004, 223, 159-167.	3.1	16
98	Influence of pH on the sorption behaviour of uranyl ions in mesoporous MCM-41 and MCM-48 molecular sieves. Materials Research Bulletin, 2004, 39, 2035-2048.	2.7	63
99	Catalytic hydrodehalogenation of aryl halides, reduction of nitroarenes and reductive cleavage of azo compounds over mesoporous Pd/MCM-41 molecular sieves under transfer hydrogenation conditions. Applied Catalysis B: Environmental, 2004, 49, 251-255.	10.8	31
100	Uranyl-anchored MCM-41 as a highly efficient photocatalyst for the complete oxidation of methanol under sunlight. Applied Catalysis B: Environmental, 2004, 54, 145-154.	10.8	28
101	Synthesis, Characterization and Catalytic Properties of Vanadium Substituted Hexagonal Mesoporous Aluminophosphate Molecular Sieves. Catalysis Letters, 2004, 93, 47-53.	1.4	9
102	Tertiary butylation of phenol over mesoporous MeMCM-48 and MeMCM-41 (Me = Ga, Fe, Al or B) solid acid catalysts. Catalysis Today, 2004, 96, 135-141.	2.2	41
103	Sunlight-Assisted Photocatalytic Oxidation of Methane over Uranyl-Anchored MCM-41. Catalysis Letters, 2004, 98, 113-116.	1.4	25
104	Chemoselective Reduction of $\hat{\Gamma}$ , $\hat{\Gamma}$ -Unsaturated Carbonyls over Novel Mesoporous CoHMA Molecular Sieves under Hydrogen Transfer Conditions. Advanced Synthesis and Catalysis, 2004, 346, 542-544.	2.1	44
105	Chemo- and Regioselective Reduction of Nitroarenes, Carbonyls and Azo Dyes over Nickel-Incorporated Hexagonal Mesoporous Aluminophosphate Molecular Sieves.. ChemInform, 2004, 35, no.	0.1	0
106	Selective Oxidation of Cycloalkanes over Iron-Substituted Hexagonal Mesoporous Aluminophosphate Molecular Sieves.. ChemInform, 2004, 35, no.	0.1	0
107	Selective Reduction of Alkenes, $\hat{\Gamma}$ , $\hat{\Gamma}$ -Unsaturated Carbonyl Compounds, Nitroarenes, Nitroso Compounds, N,N-Hydrogenolysis of Azo and Hydrazo Functions as well as Simultaneous Hydrodehalogenation and Reduction of Substituted Aryl Halides over Pd/MCM-41 Catalyst under Transfer Hydrogen Conditions.. ChemInform, 2004, 35, no.	0.1	0
108	Theoretical Calculations on Electronic Structure and Catalytic Reaction of Organo-f-Element Complexes. ChemInform, 2004, 35, no.	0.1	0



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109	Periodic density functional investigation of Brønsted acidity in isomorphously substituted chabazite and AlPO-34 molecular sieves. <i>Microporous and Mesoporous Materials</i> , 2004, 71, 51-56.	2.2	35
110	Synthesis, characterization and catalytic properties of mesoporous TiHMA molecular sieves: selective oxidation of cycloalkanes. <i>Microporous and Mesoporous Materials</i> , 2004, 73, 137-149.	2.2	20
111	Mesoporous VMCM-41: highly efficient and remarkable catalyst for selective oxidation of cyclohexane to cyclohexanol. <i>Journal of Molecular Catalysis A</i> , 2004, 223, 241-250.	4.8	55
112	A theoretical study on the cyclopropane adsorption onto the copper surfaces by density functional theory and quantum chemical molecular dynamics methods. <i>Journal of Molecular Catalysis A</i> , 2004, 220, 189-198.	4.8	21
113	Chemo- and regioselective reduction of nitroarenes, carbonyls and azo dyes over nickel-incorporated hexagonal mesoporous aluminophosphate molecular sieves. <i>Tetrahedron Letters</i> , 2004, 45, 2003-2007.	0.7	37
114	Selective reduction of alkenes, $\hat{1}\pm, \hat{1}^2$ -unsaturated carbonyl compounds, nitroarenes, nitroso compounds, N,N-hydrogenolysis of azo and hydrazo functions as well as simultaneous hydrodehalogenation and reduction of substituted aryl halides over PdMCM-41 catalyst under transfer hydrogen conditions. <i>Tetrahedron Letters</i> , 2004, 45, 3071-3075.	0.7	59
115	Electronic structure of the electrode/electrolyte interface: large-scale tight-binding quantum chemical simulation. <i>Solid State Ionics</i> , 2004, 175, 847-850.	1.3	4
116	Mesoporous H-GaMCM-48: A remarkable solid acid catalyst for tertiary butylation of phenol. <i>Journal of Catalysis</i> , 2004, 224, 178-186.	3.1	39
117	Ligand effect on the periodic properties of trivalent organolanthanide complexes: a density functional study. <i>Inorganic Chemistry Communication</i> , 2004, 7, 566-568.	1.8	6
118	Catalytic activity of highly ordered mesoporous VMCM-48. <i>Applied Catalysis A: General</i> , 2004, 276, 257-265.	2.2	52
119	Selective Oxidation of Cycloalkanes over Iron-substituted Hexagonal Mesoporous Aluminophosphate Molecular Sieves. <i>Chemistry Letters</i> , 2004, 33, 198-199.	0.7	11
120	Theoretical Calculations on Electronic Structure and Catalytic Reaction of Organo-f-element Complexes. <i>Chemistry Letters</i> , 2004, 33, 780-785.	0.7	16
121	Title is missing!. <i>Tribology Letters</i> , 2003, 15, 155-162.	1.2	11
122	Title is missing!. <i>Topics in Catalysis</i> , 2003, 22, 17-22.	1.3	19
123	Title is missing!. <i>Catalysis Letters</i> , 2003, 85, 217-222.	1.4	24
124	Quantum Chemical Molecular Dynamics Simulation of the Plasma Etching Processes. <i>Japanese Journal of Applied Physics</i> , 2003, 42, 1859-1864.	0.8	40
125	Reductive cleavage of azo dyes and reduction of nitroarenes over trivalent iron incorporated hexagonal mesoporous aluminophosphate molecular sieves. <i>Applied Catalysis B: Environmental</i> , 2003, 46, 155-163.	10.8	35
126	Heterogeneous Catalytic Transfer Hydrogenation of Aromatic Nitro and Carbonyl Compounds over Cobalt(II) Substituted Hexagonal Mesoporous Aluminophosphate Molecular Sieves.. <i>ChemInform</i> , 2003, 34, no.	0.1	0



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127	Regio- and Chemoselective Catalytic Transfer Hydrogenation of Aromatic Nitro and Carbonyl as Well as Reductive Cleavage of Azo Compounds over Novel Mesoporous NiMCM-41 Molecular Sieves.. ChemInform, 2003, 34, no.	0.1	0
128	Catalytic Transfer Hydrogenation of Nitro and Carbonyl Compounds over Novel Fe(III) Substituted Hexagonal Mesoporous Aluminophosphates.. ChemInform, 2003, 34, no.	0.1	0
129	Quantum-chemical study on the supported precious metal catalyst. Catalysis Today, 2003, 87, 43-50.	2.2	21
130	The influence of aluminium sources on the acidic behaviour as well as on the catalytic activity of mesoporous H-AlMCM-41 molecular sieves. Microporous and Mesoporous Materials, 2003, 65, 177-187.	2.2	111
131	Density functional study of lanthanide complexes $(\eta^5\text{-C}_5\text{H}_5)_2\text{LnX}^{\text{OC}_4\text{H}_8}$ (Ln=La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu; X=F, Cl, Br and I). Journal of Organometallic Chemistry, 2003, 679, 84-92.	0.8	16
132	Theoretical investigation of mixed-ligand lanthanocene complexes, $(\eta^5\text{-C}_5\text{H}_5)_2\text{LnX}^{\text{OC}_4\text{H}_8}$ (Ln=La, Gd, Lu; X=F, Cl, Br, I). Journal of Organometallic Chemistry, 2003, 679, 93-100.	1.8	11
133	Allylic oxidation of cyclohexene over chromium containing mesoporous molecular sieves. Applied Catalysis A: General, 2003, 246, 283-293.	2.2	89
134	Monte Carlo simulation of hydrogen absorption in palladium and palladium-silver alloys. Catalysis Today, 2003, 82, 233-240.	2.2	8
135	Mesoporous H-AlMCM-48: highly efficient solid acid catalyst. Applied Catalysis A: General, 2003, 254, 239-249.	2.2	42
136	Novel mesoporous (Cr)MCM-48 molecular sieves: Promising heterogeneous catalysts for selective oxidation reactions. New Journal of Chemistry, 2003, 27, 1184.	1.4	67
137	A Quantum Molecular Dynamics Simulation Study of the Initial Hydrolysis Step in Sol-Gel Process. Journal of Physical Chemistry B, 2003, 107, 1518-1524.	1.2	115
138	Density Functional Study of the Insertion and Ring-Opening Mechanism of MCP over Cp <sub>2</sub> LaH and Cp <sub>2</sub> LuH Catalysts. Journal of the American Chemical Society, 2003, 125, 16210-16212.	6.6	13
139	Ring Opening of Methylene cyclopropane over Lanthanocene Catalyst: A Quantum-Chemical Molecular Dynamics Simulation Study. Organometallics, 2003, 22, 2181-2183.	1.1	35
140	Titanium substituted hexagonal mesoporous aluminophosphates: Highly efficient and selective heterogeneous catalysts for the oxidation of phenols at room temperature. Catalysis Communications, 2003, 4, 57-62.	1.6	33
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