

# Alireza Najafi Chermahini

## List of Publications by Year in descending order

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156  
papers

3,073  
citations

186265

28  
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223800

46  
g-index

161  
all docs

161  
docs citations

161  
times ranked

3495  
citing authors

#	ARTICLE	IF	CITATIONS
1	Direct production of hydrogen peroxide over bimetallic CoPd catalysts: Investigation of the effect of Co addition and calcination temperature. <i>Green Energy and Environment</i> , 2023, 8, 246-257.	8.7	4
2	Boron nitride nanosheets supported highly homogeneous bimetallic AuPd alloy nanoparticles catalyst for hydrogen production from formic acid. <i>Nanotechnology</i> , 2022, , .	2.6	7
3	Biomass conversion to alkyl levulinates using heteropoly acid carbon mesoporous composites. <i>Chemical Engineering Research and Design</i> , 2022, 160, 988-1000.	5.6	9
4	In situ hydrogenation of phenol using sodium formate in an aqueous medium on unmodified palladium catalysts supported on KIT-5: Investigation of calcination temperature effect. <i>Molecular Catalysis</i> , 2022, 524, 112337.	2.0	3
5	Facile synthesis of Pd@Au/BNNS bimetallic catalysts for direct generation of $H_2O_2$ from $H_2$ and $O_2$ under environmentally friendly conditions. <i>Green Chemistry</i> , 2022, 24, 5524-5534.	9.0	3
6	Dehydration of carbohydrates into 5-hydroxymethylfurfural over vanadyl pyrophosphate catalysts. <i>Renewable Energy</i> , 2021, 164, 11-22.	8.9	27
7	A new catalytic system for oxidative desulfurization of model diesel by hierarchical TiO <sub>2</sub> nanotube arrays on titanium foil. <i>Journal of Porous Materials</i> , 2021, 28, 629-640.	2.6	5
8	Application of vanadyl hydrogen phosphate/KIT-6 composites as a catalyst for dehydration of sucrose. <i>Journal of the Iranian Chemical Society</i> , 2021, 18, 2291-2302.	2.2	2
9	Fabricating boron nitride nanosheets from hexagonal BN in water solution by a combined sonication and thermal-assisted hydrolysis method. <i>Ceramics International</i> , 2021, 47, 11122-11128.	4.8	17
10	Mono lacunary phosphomolybdate supported on mesoporous graphitic carbon nitride: An eco-friendly and efficient catalyst for oxidative desulfurization of the model and real fuels. <i>Journal of Environmental Chemical Engineering</i> , 2021, 9, 105430.	6.7	12
11	Synthesis of n-butyl levulinate as a fuel additive using bimetallic Zr/Al catalysts supported on mesoporous silica: Applying experimental design to optimize the reaction conditions. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 625, 126885.	4.7	9
12	Synthesis and characterization of Pd-Ni catalysts supported on KIT-6 and their application in cyclohexane oxidation using molecular oxygen. <i>Journal of Industrial and Engineering Chemistry</i> , 2021, 102, 103-111.	5.8	15
13	Synthesis of arylhydrazone-based molecular switches using aryl diazonium silica sulfate nanocomposites and analysis of their isomerization. <i>Dyes and Pigments</i> , 2021, 194, 109544.	3.7	5
14	A comparative theoretical study of the chiral discrimination of phenylalanine enantiomers by the cyclic peptides with different sizes as discriminating agents: A DFT study. <i>Journal of Molecular Structure</i> , 2021, 1243, 130904.	3.6	3
15	Photocatalytic oxidation of benzyl alcohol and the photoelectrochemical water splitting of visible light-activated TiO <sub>2</sub> nanostructures prepared by one-step titanium anodization. <i>Applied Physics A: Materials Science and Processing</i> , 2021, 127, 1.	2.3	3
16	Direct production of hexyl levulinate as a potential fuel additive from glucose catalyzed by modified dendritic fibrous nanosilica. <i>Renewable Energy</i> , 2020, 147, 2229-2237.	8.9	18
17	Surface modification of alumina with P <sub>2</sub> O <sub>5</sub> and its application in 2-octanol dehydration. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2020, 129, 265-282.	1.7	3
18	Glycerol adsorption and mechanism of dehydration to acrolein over TiO <sub>2</sub> surface: A density functional theory study. <i>Journal of Colloid and Interface Science</i> , 2020, 563, 1-7.	9.4	22

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19	Preparation of kapa carrageenan-based acidic heterogeneous catalyst for conversion of sugars to high-value added materials. <i>International Journal of Biological Macromolecules</i> , 2020, 165, 1129-1138.	7.5	15
20	Direct conversion of xylose to butyl levulinate over mesoporous zirconium silicates with an integrated dehydration alcoholysis process. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2020, 114, 168-175.	5.3	8
21	Sulfonated CMK-3: an effective catalyst for the glucose conversion to butyl levulinate as the fuel additive. <i>Biomass Conversion and Biorefinery</i> , 2020, , 1.	4.6	4
22	A DFT study on production of hydrogen from biomass-derived formic acid catalyzed by Pt@TiO <sub>2</sub> . <i>International Journal of Hydrogen Energy</i> , 2020, 45, 20993-21003.	7.1	19
23	Synthesis of hexyl levulinate as a potential fuel additive from levulinic acid over a solid acid catalyst. <i>Journal of Environmental Chemical Engineering</i> , 2019, 7, 103420.	6.7	4
24	Lacunary phosphomolybdate PMo <sub>11</sub> supported on mesoporous KIT-6 as catalyst for oxidative desulfurization of model diesel. <i>Journal of Porous Materials</i> , 2019, 26, 1691-1698.	2.6	10
25	Production of n-butyl levulinate over modified KIT-6 catalysts: comparison of the activity of KIT-SO <sub>3</sub> H and Al-KIT-6 catalysts. <i>Journal of the Iranian Chemical Society</i> , 2019, 16, 2045-2053.	2.2	14
26	Ultra-deep desulfurization of a model fuel using novel VOHPO <sub>4</sub> /boehmite catalysts. <i>Applied Organometallic Chemistry</i> , 2019, 33, e4877.	3.5	8
27	A sulfonated triazine-based covalent organic polymer supported on a mesoporous material: a new and robust material for the production of 5-hydroxymethylfurfural. <i>Sustainable Energy and Fuels</i> , 2019, 3, 1024-1032.	4.9	38
28	VOHPO <sub>4</sub> .5H <sub>2</sub> O/KIT-6 composites: Preparation and their application in extractive and catalytic oxidation desulfurization of benzothiophene and dibenzothiophene. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2019, 97, 237-246.	5.3	27
29	Catalytic conversion of furfuryl alcohol to n-hexyl levulinate using modified dendritic fibrous nanosilica. <i>Chemical Engineering Journal</i> , 2019, 361, 450-460.	12.7	22
30	Furfural oxidation to maleic acid with H <sub>2</sub> O <sub>2</sub> by using vanadyl pyrophosphate and zirconium pyrophosphate supported on well-ordered mesoporous KIT-6. <i>Journal of Environmental Chemical Engineering</i> , 2019, 7, 102855.	6.7	27
31	The effect of the diameter of cyclic peptide nanotube on its chirality discrimination. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 691-701.	3.5	10
32	DFT and MP2 Calculations on Tautomers and Water-Assisted Proton Transfer on 1,2,5-Oxadiazol-4,3-diamine. <i>Russian Journal of Physical Chemistry A</i> , 2018, 92, 99-110.	0.6	2
33	KCC-1/Pr-SO <sub>3</sub> H as an efficient heterogeneous catalyst for production of n-butyl levulinate from furfuryl alcohol. <i>Journal of Industrial and Engineering Chemistry</i> , 2018, 62, 401-408.	5.8	36
34	KIT-6-anchored sulfonic acid groups as a heterogeneous solid acid catalyst for the synthesis of aryl tetrazoles. <i>Journal of the Iranian Chemical Society</i> , 2018, 15, 831-838.	2.2	13
35	Cyclic peptide nanocapsule as ion carrier for halides: a theoretical survey. <i>Structural Chemistry</i> , 2018, 29, 1351-1357.	2.0	3
36	Density functional theory study of carbazole dyes: Potential application of carbazole dyes in dye-sensitized solar cells. <i>Journal of Molecular Structure</i> , 2018, 1164, 155-163.	3.6	18

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37	Dehydration of fructose and glucose to 5-hydroxymethylfurfural over Al-KCC-1 silica. <i>Journal of Energy Chemistry</i> , 2018, 27, 769-780.	12.9	49
38	Fabrication and characterization of chitosan/gelatin/nanodiopside composite scaffolds for tissue engineering application. <i>Polymer Bulletin</i> , 2018, 75, 1487-1504.	3.3	7
39	Fabrication and characterization of nanobiocomposite scaffold of zein/chitosan/nanohydroxyapatite prepared by freeze-drying method for bone tissue engineering. <i>International Journal of Biological Macromolecules</i> , 2018, 108, 1017-1027.	7.5	77
40	Cleaner production of 5-hydroxymethylfurfural from fructose using ultrasonic propagation. <i>Journal of Cleaner Production</i> , 2018, 198, 381-388.	9.3	27
41	Alumina-coated mesoporous silica SBA-15 as a solid catalyst for catalytic conversion of fructose into liquid biofuel candidate ethyl levulinate. <i>Chemical Engineering Journal</i> , 2018, 352, 45-52.	12.7	41
42	The effects of second electron acceptor group on the performance of tetrazole-based nanocrystalline TiO <sub>2</sub> sensitizers in DSSCs. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 178, 79-85.	3.9	11
43	Theoretical study on the bridge comparison of TiO <sub>2</sub> nanoparticle sensitizers based on phenoxazine in dye-sensitized solar cells. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	1.4	9
44	Adsorption modes of 1,3-thiazol-2-amine on the TiO <sub>2</sub> (001) and (101) anatase surfaces. <i>Structural Chemistry</i> , 2017, 28, 1151-1162.	2.0	4
45	Green and selective oxidation of cyclohexane over vanadium pyrophosphate supported on mesoporous KIT-6. <i>Chemical Engineering Journal</i> , 2017, 314, 515-525.	12.7	49
46	The catalytic effect of Al-KIT-5 and KIT-5-SO <sub>3</sub> H on the conversion of fructose to 5-hydroxymethylfurfural. <i>Research on Chemical Intermediates</i> , 2017, 43, 5507-5521.	2.7	15
47	Transport Behavior of the Enantiomers of Lactic Acid through the Cyclic Peptide Nanotube: Enantiomer Discrimination. <i>Journal of Physical Chemistry C</i> , 2017, 121, 8165-8176.	3.1	8
48	Synthesis of new dyes containing double tetrazole groups for sensitization of TiO <sub>2</sub> nanoparticles in dye-sensitized solar cells. <i>Journal of the Iranian Chemical Society</i> , 2017, 14, 1549-1556.	2.2	4
49	Interaction of Lactic Acid and Silicon-doped Single-walled Carbon Nanotubes: A Density Functional Theory Study. <i>Journal of the Chinese Chemical Society</i> , 2017, 64, 250-260.	1.4	1
50	Esterification of the levulinic acid with n-butyl and isobutyl alcohols over aluminum-containing MCM-41. <i>Fuel Processing Technology</i> , 2017, 167, 442-450.	7.2	49
51	Theoretical study on the adsorption and relative stability of conformers of l-ascorbic acid on $\gamma$ -alumina (100) surface. <i>Journal of Molecular Structure</i> , 2017, 1147, 185-191.	3.6	4
52	Selective oxidation of toluene to benzaldehyde by H <sub>2</sub> O <sub>2</sub> with mesoporous silica KIT-6 supported VOHPO <sub>4</sub> 0.5H <sub>2</sub> O catalyst. <i>Journal of Environmental Chemical Engineering</i> , 2017, 5, 3529-3539.	6.7	22
53	Design and fabrication of novel chitin hydrogel/chitosan/nano diopside composite scaffolds for tissue engineering. <i>Ceramics International</i> , 2017, 43, 1657-1668.	4.8	34
54	A mild and highly efficient FriedlÄnder synthesis of quinolines in the presence of heterogeneous solid acid nano-catalyst. <i>Arabian Journal of Chemistry</i> , 2016, 9, S433-S439.	4.9	18

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55	A comparative MP2 study between water- and acid-assisted proton transfer: allophanic acid as a case of study. <i>Structural Chemistry</i> , 2016, 27, 1345-1362.	2.0	7
56	Chitosan /Zeolite Y/Nano ZrO <sub>2</sub> nanocomposite as an adsorbent for the removal of nitrate from the aqueous solution. <i>International Journal of Biological Macromolecules</i> , 2016, 93, 254-266.	7.5	110
57	Adsorption of some important tautomers of 5-amino tetrazole on the (001) and (101) surfaces of anatase: Theoretical study. <i>Journal of Molecular Structure</i> , 2016, 1121, 203-214.	3.6	6
58	Intermolecular interaction of guanidine and 2H-tetrazole: Enthalpy formation of guanidinium tetrazolate in the gas phase. <i>Computational and Theoretical Chemistry</i> , 2016, 1094, 42-46.	2.5	1
59	Theoretical Studies on the Adsorption of 5-Aminotetrazole on Single-walled Carbon Nanotubes. <i>Journal of the Chinese Chemical Society</i> , 2016, 63, 716-724.	1.4	1
60	Application of amine-functionalized MCM-41 as pH-sensitive nano container for controlled release of 2-mercaptobenzoxazole corrosion inhibitor. <i>Chemical Engineering Journal</i> , 2016, 306, 849-857.	12.7	71
61	Theoretical Modeling of the Chirality Discrimination of Enantiomers by Nanotubular Cyclic Peptides using Gas-Phase Photoelectron Spectroscopy: An ONIOM Spectroscopic Calculations. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6780-6791.	2.5	5
62	Density functional theory of tautomerism and water-assisted proton transfer of glycoluril. <i>Russian Journal of Physical Chemistry A</i> , 2016, 90, 1859-1868.	0.6	3
63	One-pot synthesis of ethyl(aryl)(H-tetrazol-5-yl)acrylates and (H-tetrazol-5-yl)coumarins via tandem [2+3] dipolar cycloaddition reaction-Knoevenagel condensation. <i>ChemistrySelect</i> , 2016, 1, 430-433.	1.5	4
64	Molecular Design of Carbazole-based Dyes and the Influence of Alkyl Substituent on the Performance of Dye-Sensitized Solar Cells. <i>Molecular Crystals and Liquid Crystals</i> , 2016, 629, 29-43.	0.9	2
65	Enantiomeric discrimination of leucine enantiomers by nanotubular cyclic peptides: DFT and ONIOM calculation of the absorption spectra of guested enantiomers. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2016, 85, 329-339.	1.6	5
66	Amino-functionalized mesoporous silica as solid base catalyst for regioselective aza-Michael reaction of aryl tetrazoles. <i>Journal of Porous Materials</i> , 2016, 23, 441-451.	2.6	12
67	The effect of deformation and intermolecular interaction on the absorption spectrum of 5-aminotetrazole and hydrazine: A computational molecular spectroscopy study on hydrazinium 5-aminotetrazolate. <i>Journal of Molecular Structure</i> , 2016, 1107, 121-136.	3.6	2
68	A DFT approach for simple and solvent assisted-proton movement: Biurea as a case of study. <i>Computational and Theoretical Chemistry</i> , 2016, 1084, 67-74.	2.5	9
69	Production of 5-hydroxymethylfurfural from fructose using a spherically fibrous KCC-1 silica catalyst. <i>RSC Advances</i> , 2016, 6, 33804-33810.	3.6	42
70	The catalytic conversion of fructose into 5-hydroxymethylfurfural over acid-functionalized KIT-6, an ordered mesoporous silica. <i>Chemical Engineering Journal</i> , 2016, 294, 380-388.	12.7	82
71	Theoretical study of microhydrated cyclo(L-pro)4-alkali cation complexes. <i>Computational and Theoretical Chemistry</i> , 2016, 1078, 37-46.	2.5	1
72	Comparing the ion affinity of two ionophores: Theoretical study of alkali earth metal ion-nanotubular cyclic peptide complexes. <i>Journal of Molecular Liquids</i> , 2016, 214, 101-110.	4.9	6

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73	Selective Complexation of $\text{Ca}^{2+}$ Cations with Nanotubular Silk Type Cyclopeptides: A DFT Study. <i>Journal of the Chinese Chemical Society</i> , 2015, 62, 1105-1113.	1.4	2
74	Fabrication and characterization of POM/ZrO <sub>2</sub> /silk fibroin composite scaffolds. <i>Materials Letters</i> , 2015, 157, 85-88.	2.6	8
75	Complexation of all-cis cyclo(L-Pro) <sub>3</sub> and alkali metal cations: a DFT study. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2015, 81, 465-473.	1.6	7
76	Nano-composite of silk fibroin-chitosan/Nano ZrO <sub>2</sub> for tissue engineering applications: Fabrication and morphology. <i>International Journal of Biological Macromolecules</i> , 2015, 76, 292-302.	7.5	68
77	Protein-ligand interaction study of signal transducer smoothened protein with different drugs: molecular docking and QM/MM calculations. <i>RSC Advances</i> , 2015, 5, 68829-68838.	3.6	10
78	Novel organic dyes with anchoring group of barbituric/thiobarbituric acid and their application in dye-sensitized solar cells. <i>Synthetic Metals</i> , 2015, 209, 1-10.	3.9	36
79	Dissociation, absorption and ionization of some important sulfur oxoanions ( $\text{SO}_n^{2-n}$ , n=2, 3, 4, 6, 7 and) <i>Tj ETQq</i> 1, 1 0.7843, 14 rgBT 3.6	3.6	2
80	Application of a functionalized mesoporous silica catalyst to the synthesis of tetrazoles. <i>New Journal of Chemistry</i> , 2015, 39, 4814-4820.	2.8	20
81	Fabrication and characterization of silk fibroin/chitosan/Nano $\text{Al}_2\text{O}_3$ -alumina composite scaffolds for tissue engineering applications. <i>RSC Advances</i> , 2015, 5, 27558-27570.	3.6	27
82	New tetrazole-based organic dyes for dye-sensitized solar cells. <i>Journal of Energy Chemistry</i> , 2015, 24, 770-778.	12.9	18
83	A DFT-D study on the interaction between lactic acid and single-wall carbon nanotubes. <i>RSC Advances</i> , 2015, 5, 97724-97733.	3.6	9
84	Fluorine substituent effect on the adsorption of acetic acid derivatives ( $\text{CH}_3\text{CO}_2\text{H}$ ) on anatase TiO <sub>2</sub> (1 0 0) and (1 0 1) surfaces. <i>Applied Surface Science</i> , 2015, 357, 1260-1267.	6.1	5
85	Preparation, characterization, degradation and biocompatibility of different silk fibroin based composite scaffolds prepared by freeze-drying method for tissue engineering application. <i>Polymer Degradation and Stability</i> , 2015, 121, 18-29.	5.8	56
86	Synthesis and characterization of organic dyes bearing new electron-withdrawing group for dye-sensitized solar cells. <i>Electrochimica Acta</i> , 2015, 186, 504-511.	5.2	24
87	A theoretical study on the interaction of amphetamine and single-walled carbon nanotubes. <i>Applied Surface Science</i> , 2015, 329, 87-93.	6.1	13
88	Synthesis and characterization of a chitosan/montmorillonite/ZrO <sub>2</sub> nanocomposite and its application as an adsorbent for removal of fluoride. <i>RSC Advances</i> , 2015, 5, 6771-6781.	3.6	57
89	Selective complexation of alkaline earth metal ions with nanotubular cyclopeptides: DFT theoretical study. <i>RSC Advances</i> , 2015, 5, 2305-2317.	3.6	23
90	Catalytic conversion of glucose to 5-hydroxymethylfurfural (HMF) using nano-POM/nano-ZrO <sub>2</sub> /nano- $\text{Al}_2\text{O}_3$ . <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2015, 49, 40-50.	5.3	25

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91	Metal ion binding of s-block cations and nanotubular cyclic (proline) <sub>4</sub> : A theoretical study. <i>Structural Chemistry</i> , 2015, 26, 675-684.	2.0	11
92	Silver nanoparticles with 4,4'-dicyanamidobiphenyl ligand: Synthesis, photoluminescent and electroluminescent properties and DFT calculations. <i>Journal of Molecular Structure</i> , 2015, 1082, 56-61.	3.6	8
93	Tautomerism and mechanism of intramolecular proton transfer under the gas phase and micro-hydrated solvent conditions: biuret as a case study. <i>Structural Chemistry</i> , 2015, 26, 159-169.	2.0	8
94	UV-VIS, NMR AND FT-IR SPECTRA OF TAUTOMERS OF VITAMIN C. EXPERIMENTAL AND DFT CALCULATIONS. <i>Journal of the Chilean Chemical Society</i> , 2014, 59, 2588-2594.	1.2	18
95	Selective complexation of alkali metal ions and nanotubular cyclopeptides: a DFT study. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2014, 79, 205-214.	1.6	12
96	Anti-inflammatory drugs interacting with Zn (II) metal ion based on thiocyanate and azide ligands: Synthesis, spectroscopic studies, DFT calculations and antibacterial assays. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 128, 183-190.	3.9	18
97	Theoretical studies on proton transfer reaction of 3(5)-substituted pyrazoles. <i>Journal of Chemical Sciences</i> , 2014, 126, 273-281.	1.5	13
98	A periodic density functional theory study of tetrazole adsorption on anatase surfaces: potential application of tetrazole rings in dye-sensitized solar cells. <i>Journal of Molecular Modeling</i> , 2014, 20, 2086.	1.8	10
99	DFT and MP2 Study of Intermolecular Interaction of 5-Aminotetrazole and Hydrazine: Enthalpy of Formation of Hydrazinium 5-Aminotetrazolate in the Gas Phase. <i>Propellants, Explosives, Pyrotechnics</i> , 2014, 39, 496-503.	1.6	5
100	Synthesis of triazenes by using aryl diazonium silica sulfates under mild conditions. <i>Dyes and Pigments</i> , 2014, 101, 295-302.	3.7	25
101	Theoretical studies on the reactivity of mono-substituted imidazole ligands. <i>Structural Chemistry</i> , 2014, 25, 583-592.	2.0	10
102	Characterization and catalytic properties of molybdenum oxide catalysts supported on ZrO <sub>2</sub> ·nH <sub>2</sub> O-Al <sub>2</sub> O <sub>3</sub> for ammoxidation of toluene. <i>RSC Advances</i> , 2014, 4, 37679-37686.	3.6	13
103	A complete scheme of tautomerism on diacetyl monoxime in the gas and solution phases. A comparative DFT study between B3LYP and M06-2X functionals. <i>Computational and Theoretical Chemistry</i> , 2014, 1045, 10-21.	2.5	23
104	Theoretical studies of urea adsorption on single wall boron-nitride nanotubes. <i>Applied Surface Science</i> , 2014, 320, 231-236.	6.1	23
105	Theoretical studies on the reactivity of thiazole derivatives. <i>Monatshefte für Chemie</i> , 2014, 145, 1769-1776.	1.8	3
106	Theoretical study on structure, conformation, stability and electronic transition of C4 and C5 anions of ascorbic acid stereoisomers. <i>Journal of Molecular Structure</i> , 2014, 1061, 69-75.	3.6	9
107	Fabrication and characterization of silk/forsterite composites for tissue engineering applications. <i>Ceramics International</i> , 2014, 40, 6405-6411.	4.8	25
108	Synthesis, characterization and application of various types of alumina and nano- $\gamma$ -alumina sulfuric acid for the synthesis of 2,5-disubstituted 1,3,4-oxadiazoles. <i>Acta Chimica Slovenica</i> , 2014, 61, 51-8.	0.6	4



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109	Theoretical studies on the tautomerism of tetrazole selenone. <i>Journal of Molecular Modeling</i> , 2013, 19, 4377-4386.	1.8	4
110	Enantiomeric separation of d- and l-lactic acid enantiomers by use of nanotubular cyclicpeptides: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2013, 1020, 163-169.	2.5	7
111	Theoretical studies on tautomerism of imidazole-2-selenone. <i>Structural Chemistry</i> , 2013, 24, 1215-1227.	2.0	11
112	An efficient and one-pot synthesis of benzimidazoles, benzoxazoles, benzothiazoles and quinoxalines catalyzed via nano-solid acid catalysts. <i>Journal of Molecular Catalysis A</i> , 2013, 373, 38-45.	4.8	80
113	Theoretical studies on the effect of substituent in the proton transfer reaction of 4-substituted pyrazoles. <i>Computational and Theoretical Chemistry</i> , 2013, 1008, 67-73.	2.5	17
114	Relation between the substituent effect and aromaticity in imidazole derivatives: A comparative study. <i>Computational and Theoretical Chemistry</i> , 2012, 994, 97-104.	2.5	19
115	One-pot Green Synthesis of Pyrrole Derivatives Catalyzed by Nano Sulfated Zirconia as a Solid Acid Catalyst. <i>Chinese Journal of Chemistry</i> , 2012, 30, 372-376.	4.9	22
116	Stereoselective (exo-specific) synthesis, dynamic <sup>1</sup> H NMR and quantum chemical conformational and configurational analysis of norbornene-aziridine-E-imidoyl system. <i>Journal of the Iranian Chemical Society</i> , 2012, 9, 339-348.	2.2	1
117	Application of modified clays in diazotization and azo coupling reactions in water. <i>Journal of Industrial and Engineering Chemistry</i> , 2012, 18, 826-833.	5.8	10
118	Synthesis, Crystal Structure and Conformational Studies of Schiff-Base Compound 2-[[4-(Phenyldiazenyl)Phenyl]Iminomethyl]-5-Bromophenol. <i>Journal of Chemical Crystallography</i> , 2012, 42, 136-140.	1.1	6
119	A Simple and Efficient One-Pot Three-Component Synthesis of Propargylamines Using Bismuth (III) Chloride. <i>Bulletin of the Korean Chemical Society</i> , 2012, 33, 1556-1560.	1.9	30
120	Studies on tautomerism in the triazoline dione. <i>Canadian Journal of Chemistry</i> , 2011, 89, 1387-1395.	1.1	11
121	An efficient and one-pot synthesis of 2,4,5-trisubstituted and 1,2,4,5-tetrasubstituted imidazoles catalyzed via solid acid nano-catalyst. <i>Journal of Molecular Catalysis A</i> , 2011, 346, 39-45.	4.8	123
122	MP2, DFT and ab initio calculations on thioxanthone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 82, 49-55.	3.9	16
123	Zeolite and sulfated zirconia as catalysts for the synthesis of 5-substituted 1H-tetrazoles via [2+3] cycloaddition of nitriles and sodium azide. <i>Polyhedron</i> , 2011, 30, 2606-2610.	2.2	39
124	Theoretical studies on tautomerism of tetrazole 5-thion. <i>Structural Chemistry</i> , 2011, 22, 175-181.	2.0	22
125	Synthesis of mono and bis-4-methylpiperidiniummethyl-urea as corrosion inhibitors for steel in acidic media. <i>Frontiers of Chemical Science and Engineering</i> , 2011, 5, 43-50.	4.4	9
126	Simple and efficient synthesis of 5-substituted 1H-tetrazoles using metal-modified clay catalysts. <i>Heteroatom Chemistry</i> , 2011, 22, 168-173.	0.7	45



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127	Linear free energy relationship for the anomeric effect: MP2, DFT and ab initio study of 2-substituted-1,4-dioxanes. Carbohydrate Research, 2011, 346, 1047-1056.	2.3	8
128	Theoretical Studies of Hydrogen Bond Interactions in 4-Substituted Benzoic Acids Dimers. Journal of the Korean Chemical Society, 2011, 55, 392-399.	0.2	2
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