Alireza Najafi Chermahini

List of Publications by Year
in descending order

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156	3,073	186265	223800
papers	citations	28 h-index	46 g-index

161	161	161	3495
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Experimental and CIS, TD-DFT, ab initio calculations of visible spectra and the vibrational frequencies of sulfonyl azide-azoic dyes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 72, 369-377.	3.9	128
2	An efficient and one-pot synthesis of 2,4,5-trisubstituted and 1,2,4,5-tetrasubstituted imidazoles catalyzed via solid acid nano-catalyst. Journal of Molecular Catalysis A, 2011, 346, 39-45.	4.8	123
3	Chitosan /Zeolite Y/Nano ZrO 2 nanocomposite as an adsorbent for the removal of nitrate from the aqueous solution. International Journal of Biological Macromolecules, 2016, 93, 254-266.	7.5	110
4	Green and efficient diazotization and diazo coupling reactions on clays. Dyes and Pigments, 2007, 73, 239-244.	3.7	100
5	The catalytic conversion of fructose into 5-hydroxymethylfurfural over acid-functionalized KIT-6, an ordered mesoporous silica. Chemical Engineering Journal, 2016, 294, 380-388.	12.7	82
6	An efficient and one-pot synthesis of benzimidazoles, benzoxazoles, benzothiazoles and quinoxalines catalyzed via nano-solid acid catalysts. Journal of Molecular Catalysis A, 2013, 373, 38-45.	4.8	80
7	Fabrication and characterization of nanobiocomposite scaffold of zein/chitosan/nanohydroxyapatite prepared by freeze-drying method for bone tissue engineering. International Journal of Biological Macromolecules, 2018, 108, 1017-1027.	7.5	77
8	Application of amine-functionalized MCM-41 as pH-sensitive nano container for controlled release of 2-mercaptobenzoxazole corrosion inhibitor. Chemical Engineering Journal, 2016, 306, 849-857.	12.7	71
9	Nano-composite of silk fibroinâ€“chitosan/Nano ZrO2 for tissue engineering applications: Fabrication and morphology. International Journal of Biological Macromolecules, 2015, 76, 292-302.	7.5	68
10	Rapid and efficient diazotization and diazo coupling reactions on silica sulfuric acid under solvent-free conditions. Dyes and Pigments, 2009, 81, 240-244.	3.7	61
11	Synthesis and characterization of a chitosan/montmorillonite/ZrO₂ nanocomposite and its application as an adsorbent for removal of fluoride. RSC Advances, 2015, 5, 6771-6781.	3.6	57
12	Clayâ€catalyzed synthesis of 5â€substituent 1â€Hâ€tetrazoles. Journal of Heterocyclic Chemistry, 2010, 47, 913-922.	2.6	56
13	Preparation, characterization, degradation and biocompatibility ofÂdifferent silk fibroin based composite scaffolds prepared by freeze-drying method for tissue engineering application. Polymer Degradation and Stability, 2015, 121, 18-29.	5.8	56
14	DFT and ab initio study of structure of dyes derived from 2-hydroxy and 2,4-dihydroxy benzoic acids. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 69, 449-459.	3.9	55
15	Green and selective oxidation of cyclohexane over vanadium pyrophosphate supported on mesoporous KIT-6. Chemical Engineering Journal, 2017, 314, 515-525.	12.7	49
16	Esterification of the levulinic acid with n-butyl and isobutyl alcohols over aluminum-containing MCM-41. Fuel Processing Technology, 2017, 167, 442-450.	7.2	49
17	Dehydration of fructose and glucose to 5-hydroxymethylfurfural over Al-KCC-1 silica. Journal of Energy Chemistry, 2018, 27, 769-780.	12.9	49
18	Simple and efficient synthesis of 5â€substituted 1â€Hâ€tetrazoles using metalâ€modified clay catalysts. Heteroatom Chemistry, 2011, 22, 168-173.	0.7	45

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19	Production of 5-hydroxymethylfurfural from fructose using a spherically fibrous KCC-1 silica catalyst. RSC Advances, 2016, 6, 33804-33810.	3.6	42
20	Alumina-coated mesoporous silica SBA-15 as a solid catalyst for catalytic conversion of fructose into liquid biofuel candidate ethyl levulinate. Chemical Engineering Journal, 2018, 352, 45-52.	12.7	41
21	Zeolite and sulfated zirconia as catalysts for the synthesis of 5-substituted 1H-tetrazoles via [2+3] cycloaddition of nitriles and sodium azide. Polyhedron, 2011, 30, 2606-2610.	2.2	39
22	A sulfonated triazine-based covalent organic polymer supported on a mesoporous material: a new and robust material for the production of 5-hydroxymethylfurfural. Sustainable Energy and Fuels, 2019, 3, 1024-1032.	4.9	38
23	Novel organic dyes with anchoring group of barbituric/thiobarbituric acid and their application in dye-sensitized solar cells. Synthetic Metals, 2015, 209, 1-10.	3.9	36
24	KCC-1/Pr-SO3H as an efficient heterogeneous catalyst for production of n-butyl levulinate from furfuryl alcohol. Journal of Industrial and Engineering Chemistry, 2018, 62, 401-408.	5.8	36
25	Spectroscopic, quantum chemical DFT/HF study and synthesis of [2.2.1] hept-2â€²-en-2â€²-amino-N-azatricyclo [3.2.1.02,4] octane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 71, 1749-1755.	3.9	35
26	Design and fabrication of novel chitin hydrogel/chitosan/nano diopside composite scaffolds for tissue engineering. Ceramics International, 2017, 43, 1657-1668.	4.8	34
27	A Simple and Efficient One-Pot Three-Component Synthesis of Propargylamines Using Bismuth (III) Chloride. Bulletin of the Korean Chemical Society, 2012, 33, 1556-1560.	1.9	30
28	Theoretical studies on tautomerism of tetrazole derivatives by polarisable continuum method (PCM). Computational and Theoretical Chemistry, 2007, 820, 7-11.	1.5	29
29	Synthesis, characterization, crystal structure, and theoretical studies on Schiff-base compound 6-[(5-Bromopyridin-2-yl)iminomethyl]phenol. Structural Chemistry, 2010, 21, 153-157.	2.0	29
30	Fabrication and characterization of silk fibroin/chitosan/Nano Î³-alumina composite scaffolds for tissue engineering applications. RSC Advances, 2015, 5, 27558-27570.	3.6	27
31	Cleaner production of 5-hydroxymethylfurfural from fructose using ultrasonic propagation. Journal of Cleaner Production, 2018, 198, 381-388.	9.3	27
32	VOHPO4.5H2O/KIT-6 composites: Preparation and their application in extractive and catalytic oxidation desulfurization of benzothiophene and dibenzothiphene. Journal of the Taiwan Institute of Chemical Engineers, 2019, 97, 237-246.	5.3	27
33	Furfural oxidation to maleic acid with H2O2 by using vanadyl pyrophosphate and zirconium pyrophosphate supported on well-ordered mesoporous KIT-6. Journal of Environmental Chemical Engineering, 2019, 7, 102855.	6.7	27
34	Dehydration of carbohydrates into 5-hydroxymethylfurfural over vanadyl pyrophosphate catalysts. Renewable Energy, 2021, 164, 11-22.	8.9	27
35	Synthesis of triazenes by using aryl diazonium silica sulfates under mild conditions. Dyes and Pigments, 2014, 101, 295-302.	3.7	25
36	Fabrication and characterization of silk/forsterite composites for tissue engineering applications. Ceramics International, 2014, 40, 6405-6411.	4.8	25

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37	Catalytic conversion of glucose to 5-hydroxymethylfurfural (HMF) using nano-POM/nano-ZrO2/nano-Î³-Al2O3. Journal of the Taiwan Institute of Chemical Engineers, 2015, 49, 40-50.	5.3	25
38	Synthesis, characterization, and DFT studies of a novel azo dye derived from racemic or optically active binaphthol. Tetrahedron, 2008, 64, 11776-11782.	1.9	24
39	Synthesis and characterization of organic dyes bearing new electron-withdrawing group for dye-sensitized solar cells. Electrochimica Acta, 2015, 186, 504-511.	5.2	24
40	A complete scheme of tautomerism on diacetyl monoxime in the gas and solution phases. A comparative DFT study between B3LYP and M06-2X functionals. Computational and Theoretical Chemistry, 2014, 1045, 10-21.	2.5	23
41	Theoretical studies of urea adsorption on single wall boron-nitride nanotubes. Applied Surface Science, 2014, 320, 231-236.	6.1	23
42	Selective complexation of alkaline earth metal ions with nanotubular cyclopeptides: DFT theoretical study. RSC Advances, 2015, 5, 2305-2317.	3.6	23
43	Theoretical studies on tautomerism of tetrazole 5-thion. Structural Chemistry, 2011, 22, 175-181.	2.0	22
44	Oneâ€pot Green Synthesis of Pyrrole Derivatives Catalyzed by Nano Sulfated Zirconia as a Solid Acid Catalyst. Chinese Journal of Chemistry, 2012, 30, 372-376.	4.9	22
45	Selective oxidation of toluene to benzaldehyde by H2O2 with mesoporous silica KIT-6 supported VOHPO4 0.5H2O catalyst. Journal of Environmental Chemical Engineering, 2017, 5, 3529-3539.	6.7	22
46	Catalytic conversion of furfuryl alcohol to n-hexyl levulinate using modified dendritic fibrous nanosilica. Chemical Engineering Journal, 2019, 361, 450-460.	12.7	22
47	Glycerol adsorption and mechanism of dehydration to acrolein over TiO2 surface: A density functional theory study. Journal of Colloid and Interface Science, 2020, 563, 1-7.	9.4	22
48	A new family of bis-tetrazole (BIZOL) BINOL-type ligands. Tetrahedron Letters, 2006, 47, 3929-3932.	1.4	21
49	Application of a functionalized mesoporous silica catalyst to the synthesis of tetrazoles. New Journal of Chemistry, 2015, 39, 4814-4820.	2.8	20
50	Relation between the substituent effect and aromaticity in tetrazoles, protonated tetrazoles and tetrazolate derivatives. Computational and Theoretical Chemistry, 2007, 822, 33-37.	1.5	19
51	Relation between the substituent effect and aromaticity in imidazole derivatives: A comparative study. Computational and Theoretical Chemistry, 2012, 994, 97-104.	2.5	19
52	A DFT study on production of hydrogen from biomass-derived formic acid catalyzed by Ptâ€“TiO2. International Journal of Hydrogen Energy, 2020, 45, 20993-21003.	7.1	19
53	UV-VIS, NMR AND FT-IR SPECTRA OF TAUTOMERS OF VITAMIN C. EXPERIMENTAL AND DFT CALCULATIONS. Journal of the Chilean Chemical Society, 2014, 59, 2588-2594.	1.2	18
54	Anti-inflammatory drugs interacting with Zn (II) metal ion based on thiocyanate and azide ligands: Synthesis, spectroscopic studies, DFT calculations and antibacterial assays. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 183-190.	3.9	18

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55	New tetrazole-based organic dyes for dye-sensitized solar cells. Journal of Energy Chemistry, 2015, 24, 770-778.	12.9	18
56	A mild and highly efficient FriedlÃnder synthesis of quinolines in the presence of heterogeneous solid acid nano-catalyst. Arabian Journal of Chemistry, 2016, 9, S433-S439.	4.9	18
57	Density functional theory study of carbazole dyes: Potential application of carbazole dyes in dye-sensitized solar cells. Journal of Molecular Structure, 2018, 1164, 155-163.	3.6	18
58	Direct production of hexyl levulinate as a potential fuel additive from glucose catalyzed by modified dendritic fibrous nanosilica. Renewable Energy, 2020, 147, 2229-2237.	8.9	18
59	Theoretical studies on the effect of substituent in the proton transfer reaction of 4-substituted pyrazoles. Computational and Theoretical Chemistry, 2013, 1008, 67-73.	2.5	17
60	Fabricating boron nitride nanosheets from hexagonal BN in water solution by a combined sonication and thermal-assisted hydrolysis method. Ceramics International, 2021, 47, 11122-11128.	4.8	17
61	Density functional theory study of intermolecular interactions of cyclic tetrazole dimers. Computational and Theoretical Chemistry, 2008, 867, 78-84.	1.5	16
62	Theoretical studies on tautomerism of triazole derivatives in the gas phase and solution. Computational and Theoretical Chemistry, 2010, 947, 92-100.	1.5	16
63	MP2, DFT and ab initio calculations on thioxanthone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 82, 49-55.	3.9	16
64	Theoretical studies on tautomerism of dihydropyrimidine tautomers. Computational and Theoretical Chemistry, 2008, 857, 105-110.	1.5	15
65	The catalytic effect of Al-KIT-5 and KIT-5-SO3H on the conversion of fructose to 5-hydroxymethylfurfural. Research on Chemical Intermediates, 2017, 43, 5507-5521.	2.7	15
66	Preparation of kapa carrageenan-based acidic heterogeneous catalyst for conversion of sugars to high-value added materials. International Journal of Biological Macromolecules, 2020, 165, 1129-1138.	7.5	15
67	Synthesis and characterization of Pd-Ni catalysts supported on KIT-6 and their application in cyclohexane oxidation using molecular oxygen. Journal of Industrial and Engineering Chemistry, 2021, 102, 103-111.	5.8	15
68	DFT and ab initio calculations of the vibrational frequencies and visible spectra of triazenes derived from cyclic amines. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 437-443.	3.9	14
69	DFT, ab initio and FT-IR studies of the structure of sulfonamide triazenes. Journal of the Iranian Chemical Society, 2008, 5, 74-82.	2.2	14
70	Production of n-butyl levulinate over modified KIT-6 catalysts: comparison of the activity of KIT-SO3H and Al-KIT-6 catalysts. Journal of the Iranian Chemical Society, 2019, 16, 2045-2053.	2.2	14
71	Theoretical studies on proton transfer reaction of 3(5)-substituted pyrazoles. Journal of Chemical Sciences, 2014, 126, 273-281.	1.5	13
72	Characterization and catalytic properties of molybdenum oxide catalysts supported on ZrO₂â€“Î³-Al₂O₃ for ammoxidation of toluene. RSC Advances, 2014, 4, 37679-37686.	3.6	13

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73	A theoretical study on the interaction of amphetamine and single-walled carbon nanotubes. Applied Surface Science, 2015, 329, 87-93.	6.1	13
74	KIT-6-anchored sulfonic acid groups as a heterogeneous solid acid catalyst for the synthesis of aryl tetrazoles. Journal of the Iranian Chemical Society, 2018, 15, 831-838.	2.2	13
75	Selective complexation of alkali metal ions and nanotubular cyclopeptides: a DFT study. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2014, 79, 205-214.	1.6	12
76	Amino-functionalized mesoporous silica as solid base catalyst for regioselective aza-Michael reaction of aryl tetrazoles. Journal of Porous Materials, 2016, 23, 441-451.	2.6	12
77	Mono lacunary phosphomolybdate supported on mesoporous graphitic carbon nitride: An eco-friendly and efficient catalyst for oxidative desulfurization of the model and real fuels. Journal of Environmental Chemical Engineering, 2021, 9, 105430.	6.7	12
78	Environmentally friendly efficient synthesis and mechanism of triazenes derived from cyclic amines on clays, HZSM-5 and sulfated zirconia. Applied Catalysis B: Environmental, 2007, 76, 24-33.	20.2	11
79	Studies on tautomerism in the triazoline dione. Canadian Journal of Chemistry, 2011, 89, 1387-1395.	1.1	11
80	Theoretical studies on tautomerism of imidazole-2-selenone. Structural Chemistry, 2013, 24, 1215-1227.	2.0	11
81	Metal ion binding of s-block cations and nanotubular cyclic (proline)4: A theoretical study. Structural Chemistry, 2015, 26, 675-684.	2.0	11
82	The effects of second electron acceptor group on the performance of tetrazole-based nanocrystalline TiO 2 sensitizers in DSSCs. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 178, 79-85.	3.9	11
83	Vibrational spectra and assignments using ab initio and density functional theory analysis on the structure of biotin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1516-1524.	3.9	10
84	Ab initio and DFT studies of hydrogen bond interactions in difluoroacetic acid dimer. Structural Chemistry, 2010, 21, 643-649.	2.0	10
85	Application of modified clays in diazotization and azo coupling reactions in water. Journal of Industrial and Engineering Chemistry, 2012, 18, 826-833.	5.8	10
86	A periodic density functional theory study of tetrazole adsorption on anatase surfaces: potential application of tetrazole rings in dye-sensitized solar cells. Journal of Molecular Modeling, 2014, 20, 2086.	1.8	10
87	Theoretical studies on the reactivity of mono-substituted imidazole ligands. Structural Chemistry, 2014, 25, 583-592.	2.0	10
88	Proteinâ€“ligand interaction study of signal transducer smoothened protein with different drugs: molecular docking and QM/MM calculations. RSC Advances, 2015, 5, 68829-68838.	3.6	10
89	Lacunary phosphomolybdate PMo11 supported on mesoporous KIT-6 as catalyst for oxidative desulfurization of model diesel. Journal of Porous Materials, 2019, 26, 1691-1698.	2.6	10
90	The effect of the diameter of cyclic peptide nanotube on its chirality discrimination. Journal of Biomolecular Structure and Dynamics, 2019, 37, 691-701.	3.5	10

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91	Synthesis of mono and bis-4-methylpiperidiniummethyl-urea as corrosion inhibitors for steel in acidic media. Frontiers of Chemical Science and Engineering, 2011, 5, 43-50.	4.4	9
92	Theoretical study on structure, conformation, stability and electronic transition of C4 and C5 anions of ascorbic acid stereoisomers. Journal of Molecular Structure, 2014, 1061, 69-75.	3.6	9
93	A DFT-D study on the interaction between lactic acid and single-wall carbon nanotubes. RSC Advances, 2015, 5, 97724-97733.	3.6	9
94	A DFT approach for simple and solvent assisted-proton movement: Biurea as a case of study. Computational and Theoretical Chemistry, 2016, 1084, 67-74.	2.5	9
95	Theoretical study on the bridge comparison of TiO2 nanoparticle sensitizers based on phenoxazine in dye-sensitized solar cells. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	9
96	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. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2021, 625, 126885.	4.7	9
97	Synthesis, spectroscopic characterization and DFT calculations on [4-(sulfonylazide)phenyl]-1-azide. Arkivoc, 2008, 2008, 172-187.	0.5	9
98	Biomass conversion to alkyl levulinates using heteropoly acid carbon mesoporous composites. Chemical Engineering Research and Design, 2022, 160, 988-1000.	5.6	9
99	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
100	Fabrication and characterization of POM/ZrO2/silk fibroin composite scaffolds. Materials Letters, 2015, 157, 85-88.	2.6	8
101	Silver nanoparticles with 4,4â€²-dicyanamidobiphenyl ligand: Synthesis, photoluminescent and electroluminescent properties and DFT calculations. Journal of Molecular Structure, 2015, 1082, 56-61.	3.6	8
102	Tautomerism and mechanism of intramolecular proton transfer under the gas phase and micro-hydrated solvent conditions: biuret as a case study. Structural Chemistry, 2015, 26, 159-169.	2.0	8
103	Transport Behavior of the Enantiomers of Lactic Acid through the Cyclic Peptide Nanotube: Enantiomer Discrimination. Journal of Physical Chemistry C, 2017, 121, 8165-8176.	3.1	8
104	Ultraâ€deep desulfurization of a model fuel using novel VOHPO₄ 0.5H₂O/boehmite catalysts. Applied Organometallic Chemistry, 2019, 33, e4877.	3.5	8
105	Direct conversion of xylose to butyl levulinate over mesoporous zirconium silicates with an integrated dehydration alcoholysis process. Journal of the Taiwan Institute of Chemical Engineers, 2020, 114, 168-175.	5.3	8
106	Diastereoselective formation of 18-membered ring BINOL-hydrogen phosphonate dimers - Quasi-covalent hydrogen bonds?. Canadian Journal of Chemistry, 2007, 85, 466-474.	1.1	7
107	Enantiomeric separation of d- and l-lactic acid enantiomers by use of nanotubular cyclicpeptides: A DFT study. Computational and Theoretical Chemistry, 2013, 1020, 163-169.	2.5	7
108	Complexation of all-cis cyclo(L-Pro)3 and alkali metal cations: a DFT study. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2015, 81, 465-473.	1.6	7

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109	A comparative MP2 study between water- and acid-assisted proton transfer: allophanic acid as a case of study. Structural Chemistry, 2016, 27, 1345-1362.	2.0	7
110	Fabrication and characterization of chitosan/gelatin/nanodiopside composite scaffolds for tissue engineering application. Polymer Bulletin, 2018, 75, 1487-1504.	3.3	7
111	Theoretical Studies of Hydrogen Bond Interactions in Fluoroacetic Acid Dimer. Bulletin of the Korean Chemical Society, 2010, 31, 941-948.	1.9	7
112	Boron nitride nanosheets supported highly homogeneous bimetallic AuPd alloy nanoparticles catalyst for hydrogen production from formic acid. Nanotechnology, 2022, , .	2.6	7
113	Synthesis, Crystal Structure and Conformational Studies of Schiff-Base Compound 2-{[4-(Phenyldiazenyl)Phenyl]Iminomethyl}-5-Bromophenol. Journal of Chemical Crystallography, 2012, 42, 136-140.	1.1	6
114	Adsorption of some important tautomers of 5-amino tetrazole on the (001) and (101) surfaces of anatase: Theoretical study. Journal of Molecular Structure, 2016, 1121, 203-214.	3.6	6
115	Comparing the ion affinity of two ionophores: Theoretical study of alkali earth metal ionâ€“nano tubular cyclic peptide complexes. Journal of Molecular Liquids, 2016, 214, 101-110.	4.9	6
116	DFT and MP2 Study of Intermolecular Interaction of 5â€Aminotetrazole and Hydrazine: Enthalpy of Formation of Hydrazinium 5â€Aminotetrazolate in the Gas Phase. Propellants, Explosives, Pyrotechnics, 2014, 39, 496-503.	1.6	5
117	Fluorine substituent effect on the adsorption of acetic acid derivatives (CH3â^' F CO2H) on anatase TiO2 (1 0 0) and (1 0 1) surfaces. Applied Surface Science, 2015, 357, 1260-1267.	6.1	5
118	Theoretical Modeling of the Chirality Discrimination of Enantiomers by Nanotubular Cyclic Peptides using Gas-Phase Photoelectron Spectroscopy: An ONIOM Spectroscopic Calculations. Journal of Physical Chemistry A, 2016, 120, 6780-6791.	2.5	5
119	Enantiomeric discrimination of leucine enantiomers by nanotubular cyclic peptides: DFT and ONIOM calculation of the absorption spectra of guested enantiomers. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 85, 329-339.	1.6	5
120	A new catalytic system for oxidative desulfurization of model diesel by hierarchical TiO2 nanotube arrays on titanium foil. Journal of Porous Materials, 2021, 28, 629-640.	2.6	5
121	Synthesis of arylhydrazone-based molecular switches using aryldiazonium silica sulfate nanocomposites and analysis of their isomerization. Dyes and Pigments, 2021, 194, 109544.	3.7	5
122	Aryloxy tetrazoles with axial chirality: Synthesis and partial resolution of 5-(1-(2-methoxynaphthalen-1-yl)naphthalen-2-yloxy)-1H-tetrazole. Heteroatom Chemistry, 2006, 17, 416-419.	0.7	4
123	Theoretical studies on the tautomerism of tetrazole selenone. Journal of Molecular Modeling, 2013, 19, 4377-4386.	1.8	4
124	Oneâ€“pot synthesis of ethylâ€3â€arylâ€2â€(1Hâ€tetrazolâ€5â€yl)acrylates and 3â€(1Hâ€tetrazolâ€5â€yl)coumarins via tandem [2+3] dipolar cycloaddition reactionâ€Knoevenagel condensation. ChemistrySelect, 2016, 1, 430-433.	1.5	4
125	Adsorption modes of 1,3-thiazol-2-amine on the TiO2 (001) and (101) anatase surfaces. Structural Chemistry, 2017, 28, 1151-1162.	2.0	4
126	Synthesis of new dyes containing double tetrazole groups for sensitization of TiO2 nanoparticles in dye-sensitized solar cells. Journal of the Iranian Chemical Society, 2017, 14, 1549-1556.	2.2	4

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127	Theoretical study on the adsorption and relative stability of conformers of l-ascorbic acid on Î³ -alumina (100) surface. Journal of Molecular Structure, 2017, 1147, 185-191.	3.6	4
128	Synthesis of hexyl levulinate as a potential fuel additive from levulinic acid over a solid acid catalyst. Journal of Environmental Chemical Engineering, 2019, 7, 103420.	6.7	4
129	Sulfonated CMK-3: an effective catalyst for the glucose conversion to butyl levulinate as the fuel additive. Biomass Conversion and Biorefinery, 2020, , 1.	4.6	4
130	Direct production of hydrogen peroxide over bimetallic CoPd catalysts: Investigation of the effect of Co addition and calcination temperature. Green Energy and Environment, 2023, 8, 246-257.	8.7	4
131	Design of an acidic sulfonated mesoporous carbon catalyst for the synthesis of butyl levulinate from levulinic acid. Environmental Progress and Sustainable Energy, 0, , e13721.	2.3	4
132	Synthesis, characterization and application of various types of alumina and nano-Î³-alumina sulfuric acid for the synthesis of 2,5-disubstituted 1,3,4-oxadiazoles. Acta Chimica Slovenica, 2014, 61, 51-8.	0.6	4
133	Theoretical studies on the reactivity of thiazole derivatives. Monatshefte FÃ¼r Chemie, 2014, 145, 1769-1776.	1.8	3
134	Density functional theory of tautomerism and water-assisted proton transfer of glycoluril. Russian Journal of Physical Chemistry A, 2016, 90, 1859-1868.	0.6	3
135	Cyclic peptide nanocapsule as ion carrier for halides: a theoretical survey. Structural Chemistry, 2018, 29, 1351-1357.	2.0	3
136	Surface modification of alumina with P2O5 and its application in 2-octanol dehydration. Reaction Kinetics, Mechanisms and Catalysis, 2020, 129, 265-282.	1.7	3
137	A comparative theoretical study of the chiral discrimination of phenylalanine enantiomers by the cyclic peptides with different sizes as discriminating agents: A DFT study. Journal of Molecular Structure, 2021, 1243, 130904.	3.6	3
138	Photocatalytic oxidation of benzyl alcohol and the photoelectrochemical water splitting of visible light-activated TiO2 nanostructures prepared by one-step titanium anodization. Applied Physics A: Materials Science and Processing, 2021, 127, 1.	2.3	3
139	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. Molecular Catalysis, 2022, 524, 112337.	2.0	3
140	Facile synthesis of Pdâ€“Au/BNNS bimetallic catalysts for direct generation of H₂O₂ from H₂ and O₂ under environmentally friendly conditions. Green Chemistry, 2022, 24, 5524-5534.	9.0	3
141	Asymmetric syntheses with BINOL-based imidoyl azide. Russian Journal of Organic Chemistry, 2008, 44, 1471-1477.	0.8	2
142	Selective Complexation of Sâ€block Cations with Nanotubular Silk Type Cyclopeptides: A DFT Study. Journal of the Chinese Chemical Society, 2015, 62, 1105-1113.	1.4	2
143	Dissociation, absorption and ionization of some important sulfur oxoanions (S2On2â^' n=2, 3, 4, 6, 7 and) Tj ETQq1 1 0.784314 rgBT	3.6	2
144	Molecular Design of Carbazole-based Dyes and the Influence of Alkyl Substituent on the Performance of Dye-Sensitized Solar Cells. Molecular Crystals and Liquid Crystals, 2016, 629, 29-43.	0.9	2

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145	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. Journal of Molecular Structure, 2016, 1107, 121-136.	3.6	2
146	DFT and MP2 Calculations on Tautomers and Water-Assisted Proton Transfer on 1,2,5-Oxadiazol-4,3-diamine. Russian Journal of Physical Chemistry A, 2018, 92, 99-110.	0.6	2
147	Application of vanadyl hydrogen phosphate/KIT-6 composites as a catalyst for dehydration of sucrose. Journal of the Iranian Chemical Society, 2021, 18, 2291-2302.	2.2	2
148	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
149	BENZYTRIPHENYLPHOSPHONIUM BOROHYDRIDE (BTPPB) AS A SELECTIVE REDUCING AGENT FOR REDUCTION OF IMINES, ENAMINES, AND REDUCTIVE AMINATION OF ALDEHYDES WITH PRIMARY AND SECONDRY AMINES IN METHANOL. Phosphorus, Sulfur and Silicon and the Related Elements, 2001, 170, 197-203.	1.6	1
150	Stereoselective (exo-specific) synthesis, dynamic 1H NMR and quantum chemical conformational and configurational analysis of norbornene-aziridine-E-imidoyl system. Journal of the Iranian Chemical Society, 2012, 9, 339-348.	2.2	1
151	Intermolecular interaction of guanidine and 2H-tetrazole: Enthalpy formation of guanidinium tetrazolate in the gas phase. Computational and Theoretical Chemistry, 2016, 1094, 42-46.	2.5	1
152	Theoretical Studies on the Adsorption of 5-Aminotetrazole on Single-walled Carbon Nanotubes. Journal of the Chinese Chemical Society, 2016, 63, 716-724.	1.4	1
153	Theoretical study of microhydrated cyclo(L-pro)4-alkali cation complexes. Computational and Theoretical Chemistry, 2016, 1078, 37-46.	2.5	1
154	Interaction of Lactic Acid and Siliconâ€doped Singleâ€walled Carbon Nanotubes: A Density Functional Theory Study. Journal of the Chinese Chemical Society, 2017, 64, 250-260.	1.4	1
155	Preparation of Alkyl Levulinates from Xylose Over Modified Bifunctional Mesoporous Zirconium Phosphate Catalysts. Catalysis Letters, 0, , 1.	2.6	1
156	Carrageenan-based green heterogeneous catalyst for production of 5-hydroxymethylfurfural by dehydrating fructose and glucose. Biomass Conversion and Biorefinery, 0, , 1.	4.6	1