Vithaya Ruangpornvisuti

List of Publications by Citations

129 papers	1,633 citations	19 h-index	33 g-index
132 ext. papers	1,789 ext. citations	3.2 avg, IF	5.01 L-index

#	Paper	IF	Citations
129	A-D-A sensors based on naphthoimidazoledione and boronic acid as turn-on cyanide probes in water. *Journal of Organic Chemistry*, **2009**, 74, 3919-22	4.2	100
128	Adsorption CO2 on the perfect and oxygen vacancy defect surfaces of anatase TiO2 and its photocatalytic mechanism of conversion to CO. *Applied Surface Science*, **2011**, 257, 10322-10328	6.7	87
127	Deacetylation affects the physical properties and bioactivity of acemannan, an extracted polysaccharide from Aloe vera. *Carbohydrate Polymers*, **2015**, 133, 556-66	10.3	84
126	Determination of aqueous acid-dissociation constants of aspartic acid using PCM/DFT method. *International Journal of Quantum Chemistry*, **2007**, 108, 1181-1188	2.1	81
125	Synthesis of tripodal aza crown ether calix[4]arenes and their supramolecular chemistry with transition-, alkali metal ions and anions. *Tetrahedron*, **2002**, 58, 10277-10285	2.4	67
124	Adsorption of CO, H2, N2O, NH3 and CH4 on the anatase TiO2 (001) and (101) surfaces and their competitive adsorption predicted by periodic DFT calculations. *Materials Chemistry and Physics*, **2010**, 124, 720-725	4.4	59
123	Structure and physico-chemical properties of hexadentate Schiff base zinc complexes derived from salicylaldehydes and triethylenetetramine. *Journal of Molecular Structure*, **2004**, 701, 93-103	3.4	42
122	A periodic DFT study on binding of Pd, Pt and Au on the anatase TiO2 (0 0 1) surface and adsorption of CO on the TiO2 surface-supported Pd, Pt and Au. *Applied Surface Science*, **2012**, 258, 3298-3301	6.7	37
121	Ferrocenyl derivative of 1,8-naphthalimide as a new turn-on fluorescent sensor for Au(III) ion. *Dyes and Pigments*, **2015**, 112, 236-238	4.6	36
120	Aza crown ether calix[4]arenes containing cation and anion binding sites: effects of metal ions towards anion binding ability. *Tetrahedron Letters*, **2001**, 42, 5541-5544	2	36
119	Adsorption of di-, tri- and polyatomic gases on the anatase TiO2 (0 0 1) and (1 0 1) surfaces and their adsorption abilities. *Computational and Theoretical Chemistry*, **2010**, 952, 103-108		35
118	First principles theoretical study of the hole-assisted conversion of CO to CO2 on the anatase TiO2(101) surface. *Journal of Chemical Physics*, **2011**, 134, 104701	3.9	34
117	Density functional theory investigation of the VIIIB transition metal atoms deposited on (5,5) single-walled carbon nanotubes. *Physica E: Low-Dimensional Systems and Nanostructures*, **2013**, 49, 61-67	3	31
116	Density functional investigation of hydrogen gas adsorption on Fe-doped pristine and Stone-Wales defected single-walled carbon nanotubes. *Journal of Molecular Modeling*, **2012**, 18, 3941-9	2	30
115	A DFT investigation on group 8B transition metal-doped silicon carbide nanotubes for hydrogen storage application. *Applied Surface Science*, **2018**, 439, 494-505	6.7	28
114	A density functional theory study on peptide bond cleavage at aspartic residues: direct vs cyclic intermediate hydrolysis. *Journal of Molecular Modeling*, **2013**, 19, 5501-13	2	26
113	Density functional investigation of CO adsorption on Ni-doped single-walled armchair (5,5) boron nitride nanotubes. *Journal of Molecular Modeling*, **2013**, 19, 239-45	2	23

112	First-principles investigation of adsorption of N2O on the anatase TiO2 (101) and the CO pre-adsorbed TiO2 surfaces. *Computational Materials Science*, **2012**, 58, 24-30	3.2	21
111	Recognition of carboxylate and dicarboxylates by azophenol–thiourea derivatives: a theoretical host–guest investigation. *Computational and Theoretical Chemistry*, **2004**, 686, 47-55		20
110	Adsorption of hydrogen molecule on noble metal doped on oxygen-vacancy defect of anatase TiO2(101) surface: Periodic DFT study. *International Journal of Hydrogen Energy*, **2017**, 42, 19106-19113	6.7	19
109	Conformational and energetical structures of sulfonylcalix[4]arene, p-tert-butylsulfonylcalix[4]arene and their zinc complexes. *Computational and Theoretical Chemistry* , **2003**, 629, 137-150		19
108	Theoretical study of conversion reactions of ketone to hydroxyalkylene in cluster models of zeolite H-ZSM-5. *Journal of Molecular Catalysis A*, **2005**, 239, 68-75		19
107	Acemannan increases NF-κB/DNA binding and IL-6/-8 expression by selectively binding Toll-like receptor-5 in human gingival fibroblasts. *Carbohydrate Polymers*, **2017**, 161, 149-157	10.3	18
106	Gas adsorption on the Zn-, Pd- and Os-doped armchair (5,5) single-walled carbon nanotubes. *Journal of Molecular Modeling*, **2012**, 18, 351-8	2	18
105	Molecular modeling of nitrosamines adsorbed on H-ZSM-5 zeolite: an ONIOM study. *Journal of Molecular Modeling*, **2008**, 14, 1035-41	2	18
104	Addition of diazomethane to armchair single-walled carbon nanotubes and their reaction sequences: A computational study. *Chemical Physics Letters*, **2007**, 436, 218-223	2.5	17
103	Conformational investigation of benzylhydroxamamide, its oxotechnetium(V) complexes and determination of their reaction energies. *Computational and Theoretical Chemistry*, **2004**, 676, 65-71		17
102	Synthesis of stilbene crown ether p-tert-butylcalix[4]arenes. *Tetrahedron Letters*, **2001**, 42, 5291-5293	2	17
101	Arsenite and arsenate removal from wastewater using cationic polymer-modified waste tyre rubber. *Journal of Environmental Management*, **2016**, 166, 574-8	7.9	16
100	Geometries and stabilities of transition metals doped perfect and Stone–Wales defective armchair (5,5) boron nitride nanotubes. *Structural Chemistry*, **2012**, 23, 1819-1830	1.8	16
99	Discrimination of nucleotides by single fluorescence sensor under solvent-dependent recognition patterns. *Sensors and Actuators B: Chemical*, **2012**, 171-172, 969-975	8.5	15
98	Theoretical investigation of CO2 and NO2 adsorption onto Co-, Rh- and Ir-doped (5,5) single-walled carbon nanotubes. *Materials Chemistry and Physics*, **2013**, 138, 709-715	4.4	14
97	Molecular modeling of dissociative and non-dissociative chemisorption of nitrosamine on close-ended and open-ended pristine and Stone-Wales defective (5,5) armchair single-walled carbon nanotubes. *Journal of Molecular Modeling*, **2010**, 16, 1127-38	2	14
96	A DFT investigation of conformational geometries and interconversion equilibria of phenylthiosemicarbazone and its complexation with zinc. *Journal of Molecular Modeling*, **2004**, 10, 418-26	2	14
95	Density functional studies of small gases adsorbed on the ZnO sodalite-like cage and its adsorption abilities. *Computational and Theoretical Chemistry*, **2013**, 1020, 100-107	2	13

94	Isomeric structures of benzimidazole, benzoxazole, and benzothiazole derivatives, their electronic properties and transformations. *Structural Chemistry*, **2009**, 20, 619-631	1.8	13
93	Conformational study of cationic, zwitterionic, anionic species of aspartic acid, water-added forms and their protonation. A DFT method. *Computational and Theoretical Chemistry*, **2006**, 758, 181-187		13
92	p-tert-Butylcalix[4]arene Derivatives Containing Azathiol Receptors and Their Recognition towards Hg(II). *Journal of Inclusion Phenomena and Macrocyclic Chemistry*, **2000**, 38, 113-122		13
91	Quantum chemical investigation on structures of pyrrolic amides functionalized (5,5) single-walled carbon nanotube and their binding with halide ions. *Structural Chemistry*, **2012**, 23, 7-15	1.8	12
90	A DFT study of transformation of nitrosothiol isomers and their decomposition to nitric oxide in gas phase. *International Journal of Quantum Chemistry*, **2009**, 109, 275-284	2.1	12
89	A steroid-based receptor for unprotected amino acids: the enantioselective recognition of l-tryptophan. *Tetrahedron*, **2010**, 66, 7423-7428	2.4	12
88	Synthesis of the tripodal-amine capped benzo crown p-tert-butylcalix[4]arene and its host-guest chemistry. *Tetrahedron Letters*, **1997**, 38, 3985-3988	2	12
87	Tautomeric and rotameric transformations of 4-methyl-3,6-pyridazinedione isomers. *Chemical Physics Letters*, **2005**, 415, 176-182	2.5	12
86	A density functional study of propylene glycol conversion to propanal and propanone of various acid-catalyzed reaction models: a water-addition effect. *Journal of Computational Chemistry*, **2005**, 26, 1592-9	3.5	12
85	Co-adsorptions of CO/N2O, NO/NH3, CO2/N2 and conversion of CO/N2O to CO2/N2 on ZnO graphene-like nanosheet. *Journal of Molecular Structure*, **2012**, 1012, 50-55	3.4	11
84	Fundamental insights into conformational stability and orbital interactions of antioxidant (+)-catechin species and complexation of (+)-catechin with zinc(II) and oxovanadium(IV). *Journal of Molecular Structure*, **2013**, 1047, 344-357	3.4	11
83	DFT investigation of structures of nitrosamine isomers and their transformations in gas phase. *Computational and Theoretical Chemistry*, **2006**, 766, 159-164		11
82	Molecular model for host–guest interaction of tetraamino-tert-butylthiacalix[4]arene and tetraamino-tert-butylcalix[4]arene receptors with carboxylate and dicarboxylate guests: an ONIOM study. *Journal of Molecular Modeling*, **2007**, 13, 65-77	2	11
81	Conformational structures, proton affinity of p-tert-butylthiacalix[4]arene and its zinc complex. *Computational and Theoretical Chemistry*, **2004**, 683, 103-113		11
80	Synthesis of 1,3-alternate calix[4]-cyclen-benzo-crown-6 as a hard–soft receptor. *Tetrahedron Letters*, **2000**, 41, 9167-9171	2	11
79	Discriminate sensing of pyrophosphate using a new tripodal tetramine-based dinuclear Zn(II) complex under an indicator displacement assay approach. *Dalton Transactions*, **2014**, 43, 14701-9	4.3	10
78	Theoretical Investigation of Ethanol Conversion to Ethylene over H–ZSM-5 and Transition Metals–exchanged ZSM-5. *Catalysis Letters*, **2012**, 142, 143-149	2.8	9
77	First principles investigation of oxygen adsorptions on hydrogen-terminated ZnO graphene-like nanosheets. *Journal of Molecular Modeling*, **2012**, 18, 1447-54	2	9

76	Synthesis of chromium(III) complex with 1-hydroxy-2-pyridinone-6-carboxylic acid as insulin-mimetic agent and its spectroscopic and computational studies. *Journal of Molecular Structure*, **2013**, 1031, 144-151	3.4	9
75	Inter- and intra-molecular OH stretching modes of bicarbonate in aqueous solution. *Computational and Theoretical Chemistry*, **2009**, 913, 236-239		9
74	Simultaneous removal of Ag(I), Cd(II), Cr(III), Ni(II), Pb(II), and Zn(II) from wastewater using humic acid-coated aminopropyl silica gel. *Desalination and Water Treatment*, **2016**, 57, 17411-17420		8
73	Unusual adsorption behavior of hydrogen molecules on Zr□oped perfect and oxygen□acancy defective rutile TiO2(110) surfaces: Periodic DFT study. *International Journal of Hydrogen Energy*, **2019**, 44, 32101-32111	6.7	8
72	Adsorptions of proton, hydroxide on various cap-ended and open-ended armchair (5,5) single-walled carbon nanotubes. *Chemical Physics Letters*, **2007**, 441, 127-131	2.5	8
71	Molecular structures of 3,4-dichloro-2,5-diamido-substituted pyrrole anion dimers, their deprotonation reactions in systems with and without fluoride ion. *Computational and Theoretical Chemistry*, **2006**, 772, 23-30		8
70	Structures of gas-phase nitrosamine-dimer isomers, their interconversions and energetics: A DFT study. *Computational and Theoretical Chemistry*, **2006**, 775, 113-120		8
69	Chelation behavior of various flavonols and transfer of flavonol-chelated zinc(II) to alanylaspartic dipeptide: A PCM/DFT investigation. *Journal of Molecular Structure*, **2016**, 1107, 278-290	3.4	7
68	Theoretical study on isomerization and peptide bond cleavage at aspartic residue. *Journal of Molecular Modeling*, **2013**, 19, 3627-36	2	7
67	A DFT study of chloride and hydroxide anions effects on deprotonations of 3,4-dichloro-2,5-diamido-substituted pyrrole derivatives. *Computational and Theoretical Chemistry*, **2007**, 806, 145-153		7
66	Theoretical study of adsorption of C1□3 alkoxides on various cap-ended and open-ended armchair (5,5) single-walled carbon nanotubes. *Carbon*, **2008**, 46, 12-18	10.4	7
65	A DFT investigation on molecular structures of semicarbazone complexes with Co(II), Ni(II) and Zn(II) and reaction energies of their complexation. *Structural Chemistry*, **2006**, 17, 27-34	1.8	7
64	Magnesium and lithium complexation by 1,4,7,10-tetraazacyclododecane. *Inorganica Chimica Acta*, **1988**, 144, 21-23	2.7	7
63	Substituent effect on quantum efficiency in 4-aryloxy-N-(2?,6?-diisopropylphenyl)-1,8-naphthalimides: Experimental and computational investigations. *Dyes and Pigments*, **2014**, 109, 175-180	4.6	6
62	Exploring molecular structures, orbital interactions, intramolecular proton-transfer reaction kinetics, electronic transitions and complexation of 3-hydroxycoumarin species using DFT methods. *Journal of Molecular Graphics and Modelling*, **2014**, 51, 13-26	2.8	6
61	A density functional investigation of 1,3-bis(4-nitrophenyl)urea as anion receptor. *Computational and Theoretical Chemistry*, **2009**, 902, 33-40		6
60	Conformational analysis of alkali metal complexes of anionic species of aspartic acid, their interconversion and deprotonation: a DFT investigation. *Journal of Molecular Graphics and Modelling*, **2008**, 26, 982-90	2.8	6
59	An investigation of molecular structures of sulfonylcalix[4]arene, mercaptosulfonylcalix[4]arene and aminosulfonylcalix[4]arene, their proton affinities and complexation with zinc(II). *Journal of Molecular Structure*, **2006**, 787, 76-89	3.4	6

58	Theoretical investigation of geometrical conformation, protonation of tetraamino-p-tert-butylthiacalix[4]arene and complexation with zinc: a comparative theoretical method. *Computational and Theoretical Chemistry*, **2004**, 685, 57-71		6
57	Conformational investigation of N,N?-propylene bis(benzohydroxamamide), its oxotechnetium(v) and oxorhenium(v) complexes and determination of their reaction energies. *Computational and Theoretical Chemistry*, **2005**, 755, 45-53		6
56	DFT investigation on molecular structures of metal and nonmetal-doped ZnO sodalite-like cage and their electronic properties. *Structural Chemistry*, **2016**, 27, 773-784	1.8	5
55	Self-assembly of Gd/SDS/HEPES complex and curcumin entrapment for enhanced stability, fluorescence image in cellular system. *Colloids and Surfaces B: Biointerfaces*, **2017**, 156, 254-261	6	5
54	Dipicolylamino quinoline derivative as novel dual fluorescent detecting system for Hg2+ and Fe3+. *Sensing and Bio-Sensing Research*, **2019**, 24, 100283	3.3	5
53	An ONIOM investigation of reaction mechanisms of propylene glycol dehydration over H-ZSM-5 and H-MOR catalysts. *Journal of Molecular Catalysis A*, **2012**, 363-364, 171-177		5
52	Structures and conformations of acridinium mono- and polymethine cyanine dyes and their UV□Vis absorption spectra in protic solvents: A PCM/TD-DFT study. *Journal of Molecular Structure*, **2011**, 1006, 635-641	3.4	5
51	A theoretical investigation on structures of tripodal thiourea derivatives and their anion recognition. *Structural Chemistry*, **2011**, 22, 839-847	1.8	5
50	Tryptophan receptors containing acridine-based thiourea. *Supramolecular Chemistry*, **2009**, 21, 486-494	1.8	5
49	Cation recognition of thiacalix[2]thianthrene and p-tert-butylthiacalix[2]thianthrene and their conformers and complexes with Zn(II), Cd(II) and Hg(II): a theoretical investigation. *Journal of Molecular Modeling*, **2010**, 16, 243-53	2	5
48	A DFT study of molecular structures and tautomerizations of 2-benzoylpyridine semicarbazone and picolinaldehyde N-oxide thiosemicarbazone and their complexations with Ni(II), Cu(II), and Zn(II). *Structural Chemistry*, **2007**, 18, 977-984	1.8	5
47	Anion binding of 3,4-dichloro-2,5-diamidopyrrole and anionic self-assembly dimerization of its deprotonated species. *Computational and Theoretical Chemistry*, **2008**, 864, 26-30		5
46	Recognition Studies of a Pyridine-Pendant Calix[4]arene with Neutral Molecules: Effects of Non-covalent Interactions on Supramolecular Structures and Stabilities. *Journal of Inclusion Phenomena and Macrocyclic Chemistry*, **2001**, 39, 47-53		5
45	Conformational Investigations of HMPAO Isomers and Their Zinc(II) Complexes. *Bulletin of the Korean Chemical Society*, **2002**, 23, 555-562	1.2	5
44	DFT investigation on molecular structure of zirconia nanoparticle and its adsorption structures with elementary gases. *Journal of Molecular Structure*, **2016**, 1108, 187-194	3.4	4
43	Adsorption of hydrogen and hydrogen□ontaining gases on Pd□and Ag□ingle atoms doped on anatase TiO2 (1 0 1) surfaces and their sensing performance. *Applied Surface Science*, **2018**, 450, 112-121	6.7	4
42	Theoretical study on the adsorption behaviors of H2O and NH3 on hydrogen-terminated ZnO nanoclusters and ZnO graphene-like nanosheets. *Journal of Molecular Structure*, **2011**, 994, 276-282	3.4	4
41	Molecular structures of 8,8?-dithioureido-2,2?-binaphthalene derivatives and their anions recognition: an ONIOM investigation. *Structural Chemistry*, **2009**, 20, 767-780	1.8	4

40	Isomers of various species of 1-hydroxy-2-pyridinone-6-carboxylic acid, their proton dissociation and complexes with Cr(III) and Zn(II). *Journal of Molecular Structure*, **2008**, 891, 1-10	3.4	4
39	Adsorption of sulfur-containing gases on B36 nanocluster: a DFT study. *Journal of Sulfur Chemistry*, **2021**, 42, 383-396	2.3	4
38	Highly promising discrimination of various catecholamines using ratiometric fluorescence probes with intermolecular self-association of two sensing elements. *RSC Advances*, **2015**, 5, 78468-78475	3.7	3
37	Hydrogen adsorption on Pt-decorated closed-end armchair (3,3), (4,4) and (5,5) single-walled carbon nanotubes. *Molecular Physics*, **2016**, 114, 3508-3517	1.7	3
36	Substituent effect on the proton-related phenomena and chelation behavior of hydroxypicolinic compounds: a DFT investigation. *Structural Chemistry*, **2016**, 27, 505-524	1.8	3
35	DFT investigation on adsorption of di-, tri- and tetra-atomic gases on Sc-doped ZnO sodalite like cage for gas sensing purpose. *Materials Chemistry and Physics*, **2018**, 217, 63-73	4.4	3
34	Non-rigid bis-(2,5-diamidopyrrole) receptor, its deprotonated species and their complexes with fluoride, chloride and hydroxide ions. *Computational and Theoretical Chemistry*, **2009**, 907, 131-134		3
33	Conformational analysis of alkali metal complexes of aspartate dianion and their interactions in gas phase. *Journal of Molecular Graphics and Modelling*, **2007**, 26, 342-51	2.8	3
32	Tautomerizations of 2-, 3-, and 4-formylpyridine semicarbazone conformers in gas and aqueous phases. *Structural Chemistry*, **2007**, 18, 555-561	1.8	3
31	Protonation and Energetical Investigations of Calix[4]-cyclen-benzo-crown-6 and Its Complexes with Zinc and Copper. *Bulletin of the Korean Chemical Society*, **2004**, 25, 819-822	1.2	3
30	Adsorption of propane and propylene in zeolitic imidazolate framework ZIF-8 pore: periodic SCC-DFTB method. *Adsorption*, **2018**, 24, 691-701	2.6	3
29	Hydrogen adsorption on c-ZrO2(111), t-ZrO2(101), and m-ZrO2(111) surfaces and their oxygen-vacancy defect for hydrogen sensing and storage: A first-principles investigation. *Materials Letters*, **2021**, 301, 130243	3.3	3
28	8-Hydroxyjulolidine aldimine as a fluorescent sensor for the dual detection of Al3+ and Mg2+. *Sensing and Bio-Sensing Research*, **2020**, 29, 100358	3.3	2
27	Masking Phosphate with Rare-Earth Elements Enables Selective Detection of Arsenate by Dipycolylamine-Zn Chemosensor. *Scientific Reports*, **2020**, 10, 2656	4.9	2
26	Syntheses of amide based anion receptors and investigation of their associations with anions and their molecular structures using proton NMR titration and DFT methods. *Journal of Molecular Structure*, **2014**, 1061, 32-40	3.4	2
25	IR spectroscopic and DFT investigations on molecular conformations of thio-free oxo technetium (V) benzamidoxime complexes. *Journal of Molecular Structure*, **2011**, 990, 152-157	3.4	2
24	Molecular structures and electronic properties of helical thiophene carbon-sulfur oligomers, H2(C2S) n C2H2 (n = 1-10). *Structural Chemistry*, **2010**, 21, 715-725	1.8	2
23	On the additivity of intermolecular potential functions in ion/neutral-molecule interactions. *International Journal of Mass Spectrometry and Ion Processes*, **1986**, 71, 283-286		2

22	The Interaction of Magnesium Cyclen Complex with Water. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **1987**, 42, 871-874	1.4	2
21	. *ScienceAsia*, **2002**, 28, 25	1.4	2
20	. *ScienceAsia*, **2003**, 29, 45	1.4	2
19	Hydrogen boride nanotubes and their C, N, O decoration and doping derivatives as materials for hydrogen-containing gases storage and sensing: A SCC□DFTB study. *Vacuum*, **2021**, 187, 110140	3.7	2
18	Adsorption of nitrosamine conformers on the C24, B12N12, Be12O12 and Al12P12 nanocages and their conversion to nitrogen and water molecules: A DFT study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 127, 114506	3	2
17	A study of the transition metal doped boron nitride nanosheets as promising candidates for hydrogen and formaldehyde adsorptions. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 134, 114859	3	2
16	UV□is and theoretical studies on an ensemble of dinuclear Cu(II) complex of anthracene□based tripodal tetramine with pyrogallol red for cyanide detection and species distribution in aqueous solution. *Inorganic Chemistry Communication*, **2019**, 108, 107502	3.1	1
15	A DFT investigation of dissociation of nitrous acid, transformation of its monomeric isomers, their dimeric isomers, and dimerization. *International Journal of Quantum Chemistry*, **2010**, 110, 1019-1029	2.1	1
14	Molecular structures of 3,6-di(hexylthioureido)acridine conformers, their protonation, 1H NMR and IR analyses: Theoretical and experimental studies. *Journal of Molecular Structure*, **2007**, 832, 16-25	3.4	1
13	A Monte Carlo study on the hydration of a macrocyclic magnesium complex. *Inorganica Chimica Acta*, **1987**, 134, 297-302	2.7	1
12	Effects of amino proton and denticity of quinoline-pyridine based dyes on Cd2+ and Zn2+ fluorescence sensing properties. *Journal of Photochemistry and Photobiology A: Chemistry*, **2021**, 415, 113307	4.7	1
11	A DFT study of structures of dipicolyl urea isomers and their recognition with carboxylic acids and their carboxylate anions. *Journal of Physical Organic Chemistry*, **2011**, 24, 92-100	2.1	0
10	Adsorption of hydrogen molecule on alkali metal-decorated hydrogen boride nanotubes: A DFT study. *International Journal of Hydrogen Energy*, **2021**, 46, 39273-39273	6.7	0
9	Theoretical and experimental investigations of a gold nanosensor based on rhodamine-modified carbon nanotubes. *Journal of Molecular Structure*, **2022**, 1260, 132765	3.4	0
8	Existence of □mangostin conformers and effects of aprotic and protic solvents on their equilibria, UV□Vis spectra, and chemical descriptors: Density functional theory and time-dependent density functional theory study. *Journal of Physical Organic Chemistry*, **2020**, 33, e4080	2.1	
7	First-principles investigation of ZnO sodalite-like cage binding onto TiO2 (001) surface and its ability for CO oxidation to CO2. *Journal of Materials Science*, **2014**, 49, 7620-7624	4.3	
6	An ONIOM investigation on anion recognition of alkali-metal complexes with diurea calix[4]arene receptor. *Journal of Molecular Modeling*, **2012**, 18, 2613-20	2	
5	Structural and conformational investigations of chiral bis(phenylamido)ferrocenes by X-ray crystallography and density functional calculations. *Journal of Molecular Structure*, **2009**, 938, 117-124	3.4	

List of Publications

4	A Monte Carlo Study on a Magnesium Cyclen Complex. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **1988**, 43, 797-800	1.4
3	Tautomeric transformation of temozolomide, their proton affinities and chemical reactivities: A theoretical approach. *Journal of Molecular Graphics and Modelling*, **2016**, 66, 76-84	2.8
2	A DFT calculation on nonenzymatic degradation of isoaspartic residue. *Journal of Molecular Modeling*, **2021**, 27, 300	2
1	A DFT investigation of lithium adsorption on carbonaceous compounds as a potential anode material in lithium-ion batteries. *Journal of Molecular Structure*, **2022**, 1265, 133384	3.4