AssocâEProfâEDr Hossein Farrokhpour

List of Publications by Year
in descending order

177 papers	2,012 citations	257357 24 h-index	377752 34 g-index
177 all docs	177 docs citations	177 times ranked	2333 citing authors

#	Article	IF	Citations
1	Facile and green synthesis of copper nanoparticles loaded on the amorphous carbon nitride for the oxidation of cyclohexane. Chemical Engineering Journal, 2019, 370, 1310-1321.	6.6	76
2	Immobilization of gold nanoparticles on folate-conjugated dendritic mesoporous silica-coated reduced graphene oxide nanosheets: a new nanoplatform for curcumin pH-controlled and targeted delivery. Soft Matter, 2018, 14, 2400-2410.	1.2	64
3	Theoretical studies on the potentials of some nanocages (Al12N12, Al12P12, B12N12, Be12O12, C12Si12,) Tj ETQq1 1 0.784314 rgBT / of Molecular Liquids, 2018, 260, 138-148.	2.3	58
4	Au-Pd@g-C₃N₄ as an Efficient Photocatalyst for Visible-Light Oxidation of Benzene to Phenol: Experimental and Mechanistic Study. Journal of Physical Chemistry C, 2018, 122, 27477-27485.	1.5	58
5	DFT and TD-DFT study of the adsorption and detection of sulfur mustard chemical warfare agent by the C 24 , C 12 Si 12 , Al 12 N 12 , Al 12 P 12 , Be 12 O 12 , B 12 N 12 and Mg 12 O 12 nanocages. Journal of Molecular Structure, 2018, 1164, 227-238.	1.8	52
6	Synthesis, structure, DNA/protein binding, and cytotoxic activity of a rhodium(III) complex with 2,6-bis(2-benzimidazolyl)pyridine. European Journal of Medicinal Chemistry, 2017, 127, 958-971.	2.6	46
7	Adsorption of small gas molecules on B36 nanocluster. Journal of Chemical Sciences, 2015, 127, 2029-2038.	0.7	44
8	A highly selective fluorescence turn-on chemosensor for Zn²⁺, and its application in live cell imaging, and as a colorimetric sensor for Co²⁺: experimental and TD-DFT calculations. New Journal of Chemistry, 2018, 42, 12595-12606.	1.4	42
9	SBA-15-Supported Imidazolium Ionic Liquid through Different Linkers as a Sustainable Catalyst for the Synthesis of Cyclic Carbonates: A Kinetic Study and Theoretical DFT Calculations. Industrial & Engineering Chemistry Research, 2020, 59, 12632-12644.	1.8	42
10	Imine-Linked Covalent Organic Framework with a Naphthalene Moiety as a Sensitive Phosphate Ion Sensing. ACS Applied Materials & Interfaces, 2022, 14, 22398-22406.	4.0	39
11	Ag/Pd core-shell nanoparticles by a successive method: Pulsed laser ablation of Ag in water and reduction reaction of PdCl2. Applied Surface Science, 2014, 292, 892-897.	3.1	38
12	A single chemosensor with combined ionophore/fluorophore moieties acting as a fluorescent â€œOff-Onâ€•Zn 2+ sensor and a colorimetric sensor for Cu 2+ : Experimental, logic gate behavior and TD-DFT calculations. Sensors and Actuators B: Chemical, 2017, 250, 647-658.	4.0	36
13	Description of adenine and cytosine on Au(111) nano surface using different DFT functionals (PW91PW91, wB97XD, M06-2X, M06-L and CAM-B3LYP) in the framework of ONIOM scheme: Non-periodic calculations. Chemical Physics, 2017, 488-489, 1-10.	0.9	36
14	In situ generation of the gold nanoparticlesâ€“bovine serum albumin (AuNPsâ€“BSA) bioconjugated system using pulsed-laser ablation (PLA). Materials Chemistry and Physics, 2016, 177, 360-370.	2.0	34
15	Green, efficient and large-scale synthesis of benzimidazoles, benzoxazoles and benzothiazoles derivatives using ligand-free cobalt-nanoparticles: as potential anti-estrogen breast cancer agents, and study of their interactions with estrogen receptor by molecular docking. RSC Advances, 2015, 5, 107822-107828.	1.7	33
16	Synthesis and spectroscopic characterization study of new palladium complexes containing bioactive O,O-chelated ligands: evaluation of the DNA/protein BSA interaction, in vitro antitumoural activity and molecular docking. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3324-3340.	2.0	33
17	DFT, CBSâ€Q, W1BD and G4MP2 calculation of the proton and electron affinities, gas phase basicities and ionization energies of saturated and unsaturated carboxylic acids (C₁â€“C₄). International Journal of Quantum Chemistry, 2013, 113, 1717-1721.	1.0	32
18	A rare dihydroxo copper(<scp>ii</scp>) complex with ciprofloxacin; a combined experimental and ONIOM computational study of the interaction of the complex with DNA and BSA. RSC Advances, 2014, 4, 35390.	1.7	32

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19	Photoreduction of CO₂ to CO by a mononuclear Re(<scp>i</scp>) complex and DFT evaluation of the photocatalytic mechanism. RSC Advances, 2015, 5, 41125-41134.	1.7	30
20	Experimental and theoretical spectroscopic study and structural determination of nickel(II) tridentate Schiff base complexes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 150, 220-229.	2.0	29
21	Interaction of different types of nanocages (Al₁₂N₁₂,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 672 T ClCN: DFT, TD-DFT, QTAIM, and NBO calculations. Molecular Physics, 2020, 118, 1626506.	0.8	29
22	Direct Fabrication of Au/Pd(II) Colloidal Core-Shell Nanoparticles by Pulsed Laser Ablation of Gold in PdCl₂ Solution. Journal of Physical Chemistry C, 2015, 119, 9534-9542.	1.5	28
23	Regioselective Heck reaction catalyzed by Pd nanoparticles immobilized on DNA-modified MWCNTs. RSC Advances, 2016, 6, 59124-59130.	1.7	26
24	Theoretical and Experimental Study of Valence Photoelectron Spectrum of <scp>d</scp>,<scp>l</scp>-Alanine Amino Acid. Journal of Physical Chemistry A, 2012, 116, 7004-7015.	1.1	25
25	Investigation of simultaneous formation of nano-sized CuO and ZnO on the thermal decomposition of ammonium perchlorate for composite solid propellants. Journal of Thermal Analysis and Calorimetry, 2018, 132, 879-893.	2.0	24
26	Photoelectron Spectra of Some Important Biological Molecules: Symmetry-Adapted-Cluster Configuration Interaction Study. Journal of Physical Chemistry B, 2013, 117, 6027-6041.	1.2	23
27	Selective complexation of alkaline earth metal ions with nanotubular cyclopeptides: DFT theoretical study. RSC Advances, 2015, 5, 2305-2317.	1.7	23
28	Effect of Hydration on the Kinetics of Proton-Bound Dimer Formation: Experimental and Theoretical Study. Journal of Physical Chemistry A, 2014, 118, 7663-7671.	1.1	22
29	Design of novel potential aromatase inhibitors via hybrid pharmacophore approach: docking improvement using the QM/MM method. RSC Advances, 2015, 5, 58055-58064.	1.7	21
30	Fabrication of tungsten-iron-doped TiO2 nanotubes via anodization: new photoelectrodes for photoelectrochemical cathodic protection under visible light. SN Applied Sciences, 2019, 1, 1.	1.5	21
31	An experimental and theoretical study on the interaction of DNA and BSA with novel Ni 2+ , Cu 2+ and VO 2+ complexes derived from vanillin bidentate Schiff base ligand. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 180, 144-153.	2.0	20
32	Humidity Effect on the Drift Times of the Reactant Ions in Ion Mobility Spectrometry. Analytical Chemistry, 2019, 91, 15932-15940.	3.2	20
33	Theoretical study of valance photoelectron spectra of hypoxanthine, xanthine, and caffeine using direct symmetryâ€adapted cluster/configuration interaction methodology. Journal of Computational Chemistry, 2011, 32, 2479-2491.	1.5	19
34	Ab initio intermolecular potential energy surfaces of Heâ€“CS₂, Neâ€“CS₂ and Arâ€“CS₂ complexes. Molecular Physics, 2013, 111, 779-791.	0.8	19
35	Computational and experimental study on the electrocatalytic reduction of CO2 to CO by a new mononuclear ruthenium(ii) complex. Dalton Transactions, 2014, 43, 11317.	1.6	19
36	Electrocatalytic reduction of CO₂ to CO by a mononuclear ruthenium(<scp>ii</scp>) complex. New Journal of Chemistry, 2016, 40, 6347-6357.	1.4	17

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37	Ionization energies and photoelectron spectra of fat-soluble vitamins in the gas phase: a theoretical study. RSC Advances, 2014, 4, 35975-35987.	1.7	16
38	G4MP2, DFT and CBS-Q calculation of proton and electron affinities, gas phase basicities and ionization energies of hydroxylamines and alkanolamines. Journal of Chemical Sciences, 2014, 126, 1209-1215.	0.7	16
39	Immobilization of cobalt(III) Schiff base complexes onto Montmorillonite-K10: Synthesis, experimental and theoretical structural determination. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1582-1592.	2.0	16
40	A Differential Pulse Voltammetric Sensor for Determination of Glutathione in Real Samples Using a Trichloro(terpyridine)ruthenium(III)/Multiwall Carbon Nanotubes Modified Paste Electrode. IEEE Sensors Journal, 2015, 15, 483-490.	2.4	16
41	An experimental and quantum chemical study on the non-covalent interactions of a cyclometallated Rh(<scp>iii</scp>) complex with DNA and BSA. RSC Advances, 2016, 6, 23913-23929.	1.7	16
42	Electrocatalytic reduction of CO2 to CO in the presence of a mononuclear polypyridyl ruthenium(II) complex. Journal of CO2 Utilization, 2017, 17, 80-89.	3.3	16
43	In situ synthesis of carbon nanotube-encapsulated cobalt nanoparticles by a novel and simple chemical treatment process: efficient and green catalysts for the Heck reaction. New Journal of Chemistry, 2019, 43, 8215-8219.	1.4	16
44	Experimental and ONIOM computational evaluation of DNA- and BSA-binding and cytotoxic activity of a mononuclear Pd(II) complex with piroxicam. Inorganica Chimica Acta, 2016, 453, 415-429.	1.2	15
45	Intermolecular potential energy surface for CS₂ dimer. Journal of Computational Chemistry, 2011, 32, 797-809.	1.5	14
46	Acidity constants of some sulfur oxoacids in aqueous solution using CCSD and MP2 methods. Dalton Transactions, 2013, 42, 5566.	1.6	14
47	A naphthylamide based fluorescent probe for detection of Al3+, Fe3+, and CNâ^' with high sensitivity and selectivity. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 228, 117753.	2.0	14
48	Bis- and tris(2,3-dihydro-4a,12b-(epoxyethanooxy)[1,4]dioxino[2,3-f][1,10]phenanthroline) complexes of Ru(II): Synthesis, structure and DNA binding properties. Journal of Molecular Structure, 2013, 1040, 98-111.	1.8	13
49	Theoretical study on the mechanism and kinetics of atmospheric reactions NH2OH + OOH and NH2CH3 + OOH. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 777-784.	0.9	13
50	Ionization of vitamin C in gas phase: Theoretical study. Journal of Photochemistry and Photobiology B: Biology, 2016, 160, 11-17.	1.7	13
51	Constants of explosive limits. Chemical Engineering Science, 2017, 173, 384-389.	1.9	13
52	Influence of B, Ga and In impurities in the structure and electronic properties of alumina nanoball. Chemical Physics Letters, 2010, 485, 176-182.	1.2	12
53	Urea changes oocyte competence and gene expression in resultant bovine embryo in vitro. Zygote, 2018, 26, 207-219.	0.5	12
54	ONIOM DFT study of the adsorption of cytosine on the Au/Ag and Ag/Au bimetallic nanosurfaces: The effect of sublayer. Applied Surface Science, 2018, 457, 712-725.	3.1	12

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55	Theoretical studies on tautomerism of imidazole-2-selenone. Structural Chemistry, 2013, 24, 1215-1227.	1.0	11
56	Effect of hydration on the stability and tautomerisms of different isomers of uracil. RSC Advances, 2014, 4, 61643-61651.	1.7	11
57	Linear Yukawa Isotherm Regularity for dense fluids derived based on the perturbation theory. Fluid Phase Equilibria, 2016, 409, 105-112.	1.4	11
58	Ionization of vitamin B6 in the gas phase and water: Theoretical study. Journal of Photochemistry and Photobiology A: Chemistry, 2017, 336, 77-88.	2.0	11
59	Perrhenate-Catalyzed Deoxydehydration of a Vicinal Diol: A Comparative Density Functional Theory Study. Journal of Physical Chemistry A, 2017, 121, 8688-8696.	1.1	11
60	Quantum mechanical/molecular mechanical and docking study of the novel analogues based on hybridization of common pharmacophores as potential anti-breast cancer agents. Research in Pharmaceutical Sciences, 2017, 12, 233.	0.6	11
61	Proteinâ€“ligand interaction study of signal transducer smoothened protein with different drugs: molecular docking and QM/MM calculations. RSC Advances, 2015, 5, 68829-68838.	1.7	10
62	van der Waals DFT ONIOM study of the adsorption of DNA bases on the Cu(111) nanosurface. Applied Surface Science, 2017, 422, 372-387.	3.1	10
63	The adsorption of small size Pd clusters on a g-C₃N₄ quantum dot: DFT and TD-DFT study. Materials Research Express, 2019, 6, 105079.	0.8	10
64	The effect of the diameter of cyclic peptide nanotube on its chirality discrimination. Journal of Biomolecular Structure and Dynamics, 2019, 37, 691-701.	2.0	10
65	Conformational analysis and intramolecular/intermolecular interactions of N,Nâ€²-dibenzylideneethylenediamine derivatives. Journal of Molecular Structure, 2010, 983, 169-185.	1.8	9
66	Unusual condensation of ethylene glycol with coordinated 1,10-phenanthroline-5,6-dione in [Ru(phen-dione)2Cl2] and its cyclometallated complex, [Ru(phpy-Îº2N,C2â€²)(phen-diox)2](PF6). Polyhedron, 2012, 43, 114-122.	1.0	9
67	Valence ionization of l-proline amino acid: Experimental and theoretical study. Chemical Physics Letters, 2013, 565, 102-107.	1.2	9
68	Theoretical study on ketoâ€“enol tautomerism and isomerization in pyruvic acid. International Journal of Quantum Chemistry, 2013, 113, 2372-2378.	1.0	9
69	Ab initiointermolecular potential energy surfaces for the Arâ€“NCCN van der Waals complexes. Molecular Physics, 2014, 112, 2924-2932.	0.8	9
70	Symmetry adapted clusterâ€“configuration interaction calculation of the photoelectron spectra of famous biological active steroids. Journal of Molecular Structure, 2014, 1076, 69-79.	1.8	9
71	Theoretical investigation of the borazineâ€“melamine polymer as a novel candidate for hydrogen storage applications. Physical Chemistry Chemical Physics, 2014, 16, 10519-10530.	1.3	9
72	A DFT-D study on the interaction between lactic acid and single-wall carbon nanotubes. RSC Advances, 2015, 5, 97724-97733.	1.7	9

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73	Simple and water-assisted tautomerism in succinimide. Structural Chemistry, 2015, 26, 539-545.	1.0	9
74	DFT study on the isomerization in vitamin B6. Structural Chemistry, 2014, 25, 1395-1404.	1.0	8
75	Gas phase ionization energies of some important unsaturated steroids. Structural Chemistry, 2015, 26, 71-86.	1.0	8
76	Investigation of the in situ generation of oxide-free copper nanoparticles using pulsed-laser ablation of bulk copper in aqueous solutions of DNA bases. RSC Advances, 2016, 6, 109885-109896.	1.7	8
77	Molecular thermodynamic modeling of ionic liquids using the perturbation-based linear Yukawa isotherm regularity. Journal of Physics Condensed Matter, 2016, 28, 235101.	0.7	8
78	Combined Experimental and Computational Study of the In Situ Adsorption of Piroxicam Anions on the Laser-Generated Gold Nanoparticles. Journal of Physical Chemistry C, 2017, 121, 8589-8600.	1.5	8
79	Transport Behavior of the Enantiomers of Lactic Acid through the Cyclic Peptide Nanotube: Enantiomer Discrimination. Journal of Physical Chemistry C, 2017, 121, 8165-8176.	1.5	8
80	A comparative study of the counterion effect on the perrhenate-catalyzed deoxydehydration reaction. Molecular Catalysis, 2019, 471, 27-37.	1.0	8
81	DFT investigation of endohedral boron oxide nanocapsules: Encapsulation of He, Ne, Ar, H, N, and Cl atoms. Chemical Physics, 2012, 393, 86-95.	0.9	7
82	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.	1.1	7
83	A comparative MP2 study between water- and acid-assisted proton transfer: allophanic acid as a case of study. Structural Chemistry, 2016, 27, 1345-1362.	1.0	7
84	Ionization energies, electron affinities, and binding energies of Li-doped gold nanoclusters. Research on Chemical Intermediates, 2016, 42, 4921-4936.	1.3	7
85	Average drift time and average mobility in ion mobility spectrometry. International Journal of Mass Spectrometry, 2017, 412, 20-25.	0.7	7
86	Utilization of CO2 as a carbon source for production of CO and syngas using a ruthenium(II) electrocatalyst. Journal of CO2 Utilization, 2018, 26, 612-622.	3.3	7
87	Fabrication of Pd/WO3 colloidal nanoparticles by laser ablation in liquid of tungsten for optical hydrogen detection. Journal of Laser Applications, 2019, 31, .	0.8	7
88	Study of the structural ligand effects on the fragmentation pattern of some Schiff base complexes of V (IV), Cu(II) and Ni (II) against the IR laser radiation using Matrix-free LDI-TOF technique. International Journal of Mass Spectrometry, 2019, 436, 33-41.	0.7	7
89	Directional affinity of a spherical Gold nanoparticle for the adsorption of DNA bases. Colloids and Surfaces B: Biointerfaces, 2019, 173, 493-503.	2.5	7
90	A new analytical perturbed equation of state for hard chain fluids with attractive potentials of variable range. Chemical Physics, 2008, 348, 1-10.	0.9	6

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91	Thermodynamic study of proton-bond dimers formation in atmospheric pressure: An experimental and theoretical study. Journal of Chemical Thermodynamics, 2013, 63, 17-23.	1.0	6
92	Theoretical study on the isomerization and tautomerism in barbituric acid. Structural Chemistry, 2014, 25, 1805-1810.	1.0	6
93	Theoretical study on the mechanism and kinetics of atmospheric reactions C n H2n+2Â+ÂNH2 (nÂ=Â1â€“3). Structural Chemistry, 2015, 26, 383-391.	1.0	6
94	A new force field for the adsorption of H₂, O₂, N₂, CO, H₂O, and H₂S gases on alkali doped carbon nanotubes. Molecular Physics, 2016, 114, 3375-3387.	0.8	6
95	Correlation of isothermal compressibility coefficient and reduced bulk modulus of dense fluids using perturbed linear Yukawa isotherm regularity. Physics and Chemistry of Liquids, 2017, 55, 637-649.	0.4	6
96	Fluids containing hard-chain molecules with attractive potential of variable range: Extension to mixtures and heteronuclear chain fluids. Chemical Physics, 2008, 352, 157-166.	0.9	5
97	One- and two-photon laser optogalvanic spectroscopy of neon in the 570â€“626nm region. Optics Communications, 2008, 281, 5555-5560.	1.0	5
98	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.	1.0	5
99	Ab initiointermolecular potential energy surface of NeÂ·Â·Â·NCCN van der Waals complex: effect of the place of midbond function on the interaction. Molecular Physics, 2015, 113, 3303-3311.	0.8	5
100	Structures and Photoelectron Spectra of Helium Nano Clusters. Journal of Physical Chemistry C, 2015, 119, 18641-18649.	1.5	5
101	A Simple Method for Estimating the Absolute Solvation Free Energy of Monovalent Ions in Different Solvents. Journal of Physical Chemistry A, 2015, 119, 160-171.	1.1	5
102	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.	1.1	5
103	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.	0.9	5
104	Stabilized gold nanoparticles by laser ablation in ferric chloride solutions. Applied Physics A: Materials Science and Processing, 2017, 123, 1.	1.1	5
105	A Comparative Study between Coâ€•and CoFe 2 O 4 â€NPs Catalytic Activities in Synthesis of Flavone Derivatives; Study of Their Interactions with Estrogen Receptor by Molecular Docking. ChemistrySelect, 2018, 3, 6279-6285.	0.7	5
106	Theoretical Spectroscopic Study on the Au, Ag, Au/Ag, and Ag/Au Nanosurfaces and Their Cytosine/Nanosurface Complexes: UV, IR, and Charge-Transfer SERS Spectra. Journal of Physical Chemistry C, 2019, 123, 16345-16358.	1.5	5
107	Water-vapochromic behavior of a mononuclear Pd(II) complex of piroxicam: A DFT and TD-DFT study. Journal of Molecular Graphics and Modelling, 2021, 102, 107773.	1.3	5
108	Pd/Cu-Free Cobalt-Catalyzed Suzuki and Heck Using Green Bio-Magnetic Hybrid and DFT-Based Theoretical Study. Catalysis Letters, 2021, 151, 2842-2850.	1.4	5

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109	Synthesis, X-ray structure, electrochemistry, and theoretical studies of palladium(II) complex with a tetradentate bis(quinoline-2-carboxamide) ligand. Journal of the Iranian Chemical Society, 2012, 9, 85-92.	1.2	4
110	Core photoionization of the argon dimer in the photon-energy range of 255â€“340 eV studied by a photoelectron-photoion-photoion coincidence technique. Physical Review A, 2014, 89, .	1.0	4
111	Corona discharge ionization of paracetamol molecule: Peak assignment. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 646-651.	2.0	4
112	Towards new thermodynamic regularities for dense fluids based on the effective attraction pair potential via the perturbation theory. Journal of Molecular Liquids, 2016, 220, 623-630.	2.3	4
113	Adsorption modes of 1,3-thiazol-2-amine on the TiO2 (001) and (101) anatase surfaces. Structural Chemistry, 2017, 28, 1151-1162.	1.0	4
114	Modeling the p â€“ ν â€“ T behavior of furfural compounds using perturbed linear Yukawa isotherm regularity. Journal of Molecular Liquids, 2017, 236, 18-26.	2.3	4
115	Absorption spectra of small helium Nano clusters (4He ; n= 2â€“29) and characterization of their low-lying excited states. Journal of Molecular Liquids, 2017, 230, 190-199.	2.3	4
116	Stabilization of DOPA Zwitterions on Laser-Generated Gold Nanoparticles: ONIOM Computational Study of the Charge-Dependent Structural and Electronic Changes of DOPA Adsorbed on the Gold Nanosurface. Journal of Physical Chemistry C, 2018, 122, 8680-8692.	1.5	4
117	Effect of sacrificial agents on the photoelectrochemical properties of titanium dioxide co-doped with tungsten and manganese as new visible light active. Journal of the Iranian Chemical Society, 2020, 17, 3317-3326.	1.2	4
118	Dinuclear Nickel(II) and Copper(II) Complexes of 8â€Quinolineâ€1Hâ€pyrazoleâ€3â€carboxamide: Crystal Structure, Magnetic Properties, and DFT Calculations. European Journal of Inorganic Chemistry, 2021, 2021, 1786-1795.	1.0	4
119	Thermodynamic properties of the freely jointed tangent homonuclear Yukawa chain fluid. Fluid Phase Equilibria, 2012, 313, 196-202.	1.4	3
120	Photo induced dissociation of amino acids free from thermal degradation effects: A case study applied to DL-Valine. Journal of Electron Spectroscopy and Related Phenomena, 2013, 189, 56-60.	0.8	3
121	Intramolecular H-transfer in CH2OO and cis-HO3. Structural Chemistry, 2014, 25, 1759-1763.	1.0	3
122	The excited-states intermolecular potential energy surfaces of the Arâ€“CS2 van der Waals complex: Ab initio study. Chemical Physics, 2014, 440, 8-17.	0.9	3
123	Sodium affinity of caffeine and adenine: the effect of microsolvation and electrostatic field of solvent on the sodium affinity. Molecular Physics, 2016, 114, 730-740.	0.8	3
124	Evaluation of one-dimensional potential energy surfaces for prediction of spectroscopic properties of hydrogen bonds in linear bonded complexes. Journal of Molecular Modeling, 2017, 23, 157.	0.8	3
125	Cyclic peptide nanocapsule as ion carrier for halides: a theoretical survey. Structural Chemistry, 2018, 29, 1351-1357.	1.0	3
126	Theoretical studies on the thermodynamics and kinetics of one-pot synthesis of aromatic PCP and PNP pincer ligands. Structural Chemistry, 2018, 29, 81-88.	1.0	3

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127	Extended light absorption and enhanced photoelectrochemical activity of palladiumâ€decorated hematite nanotubes prepared by photodeposition method. Applied Organometallic Chemistry, 2019, 33, e5087.	1.7	3
128	Theoretical study of the desorption of neutral and ionic alkali metal atoms from the excited Li + (H 2) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Journal of Quantum Chemistry, 2020, 120, e26104.	1.0	3
129	Surface modification of alumina with P2O5 and its application in 2-octanol dehydration. Reaction Kinetics, Mechanisms and Catalysis, 2020, 129, 265-282.	0.8	3
130	Electron affinities of X12O12 (X = Be, Mg, and Ca), X12N12 (X = B, Al, and Ga), and X12P12 (X = B, Al, and) Tj ETQq0 0 0 rgBT /Overlock 2020, 135, 1.	1.2	3
131	Excitation of hydrated Li+ and Na+ to their dissociative states: The effect of hydrogen bond on the dissociation of Li O and Na O bonds and the comparison of the TD-DFT and SAC-CI excited dissociative states. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 234, 118273.	2.0	3
132	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.	1.8	3
133	An analytical perturbed equation of state for hard chain fluids: Application to n-alkanes and n-perfluoroalkanes. Fluid Phase Equilibria, 2010, 295, 50-59.	1.4	2
134	A new simple analytical expression for the average siteâ€“site radial distribution function of hard sphere chain fluid. Fluid Phase Equilibria, 2011, 310, 90-99.	1.4	2
135	Reply to comments on â€˜Valence ionization of l-proline amino acid: Experimental and theoretical studyâ€™. Chemical Physics Letters, 2014, 601, 188-193.	1.2	2
136	Selective Complexation of Sâ€block Cations with Nanotubular Silk Type Cyclopeptides: A DFT Study. Journal of the Chinese Chemical Society, 2015, 62, 1105-1113.	0.8	2
137	Kinetics, mechanism and thermodynamics of reactions of CH₃NHNH₂ with OOH. Molecular Physics, 2015, 113, 577-583.	0.8	2
138	Kinetics, mechanism and thermodynamics of reactions of hydrazine with CH3 and OOH radicals. Research on Chemical Intermediates, 2016, 42, 1181-1194.	1.3	2
139	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.	1.8	2
140	Effect of helium nanoclusters on the spectroscopic properties of embedded SF6: Ionization, excitation and vibration. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 173, 772-782.	2.0	2
141	A Comparison of Catalytic Effect of Nanoâ€Mn₃O₄ derived from MnC₂O₄.2H₂O and Mn(acac)₃ on Thermal Decomposition of Ammonium Perchlorate. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2018, 644, 241-252.	0.6	2
142	A generalised perturbation-based equation of state for thermodynamic modelling of fluids over a wide range of density. Physics and Chemistry of Liquids, 2018, 56, 730-750.	0.4	2
143	Thermochemistry of the Reaction of Solvated Sodium Ion Clusters with Thymine in the Gas Phase: An Example of the Reaction in Microcosmic Environment. Journal of Cluster Science, 2018, 29, 521-531.	1.7	2
144	Adenine dimer on the pure and bimetallic nanosurfaces of Au and Ag metals: Hydrogen bonding on metal nanosurfaces. Computational Materials Science, 2020, 175, 109609.	1.4	2

#	Article	IF	Citations
145	Electrocatalytic property, anticancer activity, and density functional theory calculation of [NiCl(P^N^P)]Cl.EtOH. Applied Organometallic Chemistry, 2021, 35, e6092.	1.7	2
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