Mohammad Izadyar

List of Publications by Year
in descending order

154	1,744	430874	477307
papers	citations	18 h-index	29 g-index

162	162	162	1657
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Aptasensors as the future of antibiotics test kits-a case study of the aptamer application in the chloramphenicol detection. Biosensors and Bioelectronics, 2018, 122, 263-283.	10.1	124
2	A simple paper-based aptasensor for ultrasensitive detection of lead (II) ion. Analytica Chimica Acta, 2019, 1071, 70-77.	5.4	61
3	Hydrogen storage by N-ethylcarbazol as a new liquid organic hydrogen carrier: A DFT study onÂtheÂmechanism. International Journal of Hydrogen Energy, 2015, 40, 5797-5806.	7.1	50
4	Theoretical Design of Functionalized Gold Nanoparticles as Antiviral Agents against Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2). Journal of Physical Chemistry Letters, 2020, 11, 10284-10289.	4.6	45
5	Size-controlled synthesis of SnO2 nanoparticles using reverse microemulsion method. Solid State Sciences, 2014, 33, 6-11.	3.2	40
6	The role of the electronic structure and solvent in the dye-sensitized solar cells based on Zn-porphyrins: Theoretical study. Energy, 2016, 114, 559-567.	8.8	36
7	Fischerâ€“Tropsch synthesis using zeolitic imidazolate framework (ZIFâ€7 and ZIFâ€8)â€supported cobalt catalysts. Applied Organometallic Chemistry, 2020, 34, e5747.	3.5	33
8	Dissociative hydrogen adsorption on the cubic cobalt surfaces: A DFT study. International Journal of Hydrogen Energy, 2015, 40, 7064-7071.	7.1	30
9	A combined molecular dynamic and quantum mechanic study of the solvent and guest molecule effect on the stability and length of heterocyclic peptide nanotubes. Physical Chemistry Chemical Physics, 2015, 17, 11382-11391.	2.8	29
10	The investigation of the central metal effects on the porphyrin-based DSSCs performance; molecular approach. Materials Chemistry and Physics, 2017, 196, 142-152.	4.0	28
11	DFT investigation and molecular dynamic simulation on the selective complexation of cis-cyclic nanopeptides with alkaline earth metal ions. Sensors and Actuators B: Chemical, 2015, 221, 1120-1129.	7.8	27
12	Recent theoretical progress in the organic/metal-organic sensitizers as the free dyes, dye/TiO2 and dye/electrolyte systems; Structural modifications and solvent effects on their performance. Renewable and Sustainable Energy Reviews, 2018, 94, 609-655.	16.4	26
13	Efficient synthesis of novel spiro[indole-3,6â€²-pyrano[2,3-d][1,3]thiazolo[3,2-a]pyrimidine derivatives through an organobase-catalyzed, three-component reaction. Tetrahedron, 2015, 71, 2458-2462.	1.9	23
14	Anchoring Group and Ï€-Spacer Effects on the Dynamics and Kinetics of the Photovoltaic Processes in the Quinoxaline-Based Organic Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2018, 122, 23968-23977.	3.1	22
15	Evaluation and understanding the performances of various derivatives of carbonyl-stabilized phosphonium ylides in CO₂ transformation to cyclic carbonates. Physical Chemistry Chemical Physics, 2020, 22, 223-237.	2.8	21
16	Recent advances in computational methods for biosensor design. Biotechnology and Bioengineering, 2021, 118, 555-578.	3.3	20
17	A Computational Exploration of H₂S and CO₂ Capture by Ionic Liquids Based on Î±-Amino Acid Anion and N₇,N₉-Dimethyladeninium Cation. Journal of Physical Chemistry A, 2017, 121, 4352-4362.	2.5	19
18	Theoretical design and experimental study on the gold nanoparticles based colorimetric aptasensors for detection of neomycin B. Sensors and Actuators B: Chemical, 2019, 300, 126947.	7.8	19

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19	Mechanistic double ASF product distribution study of Fischerâ€“Tropsch synthesis on precipitated iron catalyst. Journal of Natural Gas Science and Engineering, 2013, 15, 53-58.	4.4	18
20	Theoretical design of the cyclic lipopeptide nanotube as a molecular channel in the lipid bilayer, molecular dynamics and quantum mechanics approach. Physical Chemistry Chemical Physics, 2015, 17, 25536-25549.	2.8	17
21	Solvent and spin state effects on molecular structure, IR spectra, binding energies and quantum chemical reactivity indices of deferiproneâ€“ferric complex: DFT study. Polyhedron, 2016, 117, 623-627.	2.2	17
22	Theoretical evaluation of the organocatalytic behavior of the negatively charged carbon atom in a fused five-member ring in carbon dioxide transformation to methanol. Energy, 2017, 134, 493-503.	8.8	17
23	Theoretical evaluation of N-alkylcarbazoles potential in hydrogen release. International Journal of Hydrogen Energy, 2017, 42, 9966-9977.	7.1	17
24	Detailed kinetics of Fischerâ€“Tropsch synthesis on a precipitated iron catalyst. Reaction Kinetics, Mechanisms and Catalysis, 2014, 111, 29-44.	1.7	16
25	A DFT study on the complex formation between desferrithiocin and metal ions (Mg2+, Al3+, Ca2+,) Tj ETQq1 1 0.784314 rgBT /Overlo	2.3	16
26	DFT study on the selective complexation of B₁₂N₁₂ nanocage with alkali metal ions. Phosphorus, Sulfur and Silicon and the Related Elements, 2018, 193, 178-184.	1.6	16
27	Theoretical design and experimental study of new aptamers with the improved target-affinity: New insights into the Pb2+-specific aptamers as a case study. Journal of Molecular Liquids, 2019, 289, 111159.	4.9	16
28	Gas-phase kinetics and mechanism of diallyl sulfide thermal decomposition. Journal of Physical Organic Chemistry, 2003, 16, 153-157.	1.9	15
29	Combination of X-ray crystallography and theoretical study to evaluate the effect of NHâ‹¯OP versus NHâ‹¯OC hydrogen bonds on the NH stretching frequencies. Journal of Molecular Structure, 2013, 1034, 354-362.	3.6	15
30	Quantum Chemistry Aspects of the Solvent Effects on 3,4-Dimethyl-2,5-dihydrothiophen-1,1-dioxide Pyrolysis Reaction. Journal of Physical Chemistry A, 2013, 117, 2427-2433.	2.5	15
31	The effect of glycosylation on the transferrin structure: A molecular dynamic simulation analysis. Journal of Theoretical Biology, 2016, 404, 73-81.	1.7	15
32	Effects of synergistic and non-synergistic anions on the iron binding site from serum transferrin: A molecular dynamic simulation analysis. Journal of Molecular Graphics and Modelling, 2017, 78, 176-186.	2.4	15
33	Modeling of the Functionalized Gold Nanoparticle Aggregation in the Presence of Dopamine: A Joint MD/QM Study. Journal of Physical Chemistry C, 2018, 122, 26130-26141.	3.1	15
34	A DFT study on the metal ion selectivity of deferiprone complexes. Computational Biology and Chemistry, 2020, 86, 107267.	2.3	15
35	First-principles study of the binding affinity of monolayer BC6N nanosheet: Implications for drug delivery. Materials Chemistry and Physics, 2022, 276, 125375.	4.0	15
36	Gas phase kinetics and mechanism of 2,2-dimethyl but-3-enal and 1-methyl-6-methylenecyclohexa-2,4-diene-1-carbaldehyde retro-cheletropic ene reaction. Computational and Theoretical Chemistry, 2004, 672, 61-66.	1.5	14

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37	Quantum chemistry aspects of the solvent effects on the ene reaction of 1-Phenyl-1,3,4-triazolin-2,5-dione and 2-methyl-2-butene. International Journal of Quantum Chemistry, 2014, 114, 666-674.	2.0	14
38	A quantum chemistry study on the performance of porphyrin-based solar cell sensitisers; Zinc and anchor group position effects. Molecular Physics, 2015, 113, 3815-3825.	1.7	14
39	The origin of regio- and stereoselectivity in the 1,3-dipolar cycloaddition of nitrile oxides with C₁-substituted 7-oxabenzonorbornadienes, a DFT study. RSC Advances, 2015, 5, 38489-38498.	3.6	14
40	Borohydride salts as high efficiency reducing reagents for carbon dioxide transformation to methanol: Theoretical approach. International Journal of Hydrogen Energy, 2016, 41, 11131-11140.	7.1	14
41	Understanding the mechanism, thermodynamic and kinetic features of the Kukhtinâ€“Ramirez reaction in carbamate synthesis from carbon dioxide. RSC Advances, 2017, 7, 1701-1710.	3.6	14
42	Highly Dispersed Palladium Nanoparticle-Loaded Magnetic Catalyst (FeS@EPâ€“AGâ€“Pd) for Suzuki Reaction in Water. Catalysis Letters, 2017, 147, 1162-1171.	2.6	14
43	Molecular engineering of the organometallic perovskites/HTMs in the PSCs: Photovoltaic behavior and energy conversion. Solar Energy Materials and Solar Cells, 2018, 180, 46-58.	6.2	14
44	Molecular dynamic simulation and DFT study on the Drug-DNA interaction; Crocetin as an anti-cancer and DNA nanostructure model. Journal of Biomolecular Structure and Dynamics, 2018, 36, 1063-1074.	3.5	14
45	Computational modeling of the photovoltaic activities in EABX3 (EAâ€¯=â€¯ethylammonium, Bâ€¯=â€¯Pb, Sn, Ge,) Ti ETQq1 1 0.78431	3.0	14
46	Advances in molecular engineering of organic-inorganic/inorganic halide perovskites: Photochemical properties behind the energy conversion ability. Solar Energy, 2019, 194, 51-60.	6.1	14
47	Structural modification as the pioneer strategy in competition of the porphyrin dye and perovskite solar cells: From dynamics to kinetics of the photovoltaic processes. Applied Physics Letters, 2019, 115, .	3.3	14
48	Substituent effects on the gas phase reactivity of alkyl allyl sulfides, a theoretical study. Computational and Theoretical Chemistry, 2006, 759, 11-15.	1.5	13
49	Diastereoselective synthesis of highly functionalized quinolizines via a pyridine-based three-component reaction and a DFT investigation on the reaction mechanism. Tetrahedron Letters, 2014, 55, 333-337.	1.4	13
50	Particle size effects in Fischer-Tropsch synthesis by Co catalyst supported on carbon nanotubes. Chinese Journal of Catalysis, 2015, 36, 1372-1378.	14.0	13
51	Improvement in charge transfer dynamic of the porphyrin-based solar cells in water: A theoretical study. Journal of Renewable and Sustainable Energy, 2017, 9, .	2.0	13
52	Sensing Ability of Hybrid Cyclic Nanopeptides Based on Thiourea Cryptands for Different Ions, A Joint DFT-D3/MD Study. Journal of Physical Chemistry A, 2017, 121, 244-255.	2.5	13
53	Glucose derivatives substitution and cyclic peptide diameter effects on the stability of the self-assembled cyclic peptide nanotubes; a joint QM/MD study. Journal of Molecular Graphics and Modelling, 2017, 71, 28-39.	2.4	13
54	A theoretical study on the efficiency and role of guanidines-based organic superbases on carbon dioxide utilization in quinazoline-2,4(1H, 3H)-diones synthesis. Structural Chemistry, 2017, 28, 675-686.	2.0	13

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55	Proton sponge as a new efficient catalyst for carbon dioxide transformation to methanol: Theoretical approach. Fuel, 2018, 221, 491-500.	6.4	13
56	The possibility of iron chelation therapy in the presence of different HPOs; a molecular approach to the non-covalent interactions and binding energies. Journal of Molecular Structure, 2018, 1166, 448-455.	3.6	13
57	A joint QM/MD study on Î±-, Î²- and Î³-cyclodextrins in selective complexation with cathinone. Supramolecular Chemistry, 2018, 30, 687-696.	1.2	13
58	Carbon Dioxide Absorption by the Imidazoliumâ€“Amino Acid Ionic Liquids, Kinetics, and Mechanism Approach. Journal of Physical Chemistry A, 2018, 122, 5721-5729.	2.5	13
59	A combined MD/QM study on the sensing mechanism of Pb2+ by glutathione functionalized gold nanoparticles. Journal of Molecular Liquids, 2019, 280, 120-127.	4.9	13
60	Photovoltaic properties of the flavonoidâ€based photosensitizers: Molecularâ€scale perspective on the natural dye solar cells. International Journal of Quantum Chemistry, 2020, 120, e26171.	2.0	13
61	A molecular dynamic study on the ability of phosphorene for designing new sensor for SARS-CoV-2 detection. Journal of Molecular Liquids, 2022, 345, 117852.	4.9	13
62	The role of solvent and structure in the kinetics of the excitons in porphyrin-based hybrid solar cells. Solar Energy, 2017, 146, 368-378.	6.1	12
63	Phosphorus ylides as a new class of compounds in CO2 activation: Thermodynamic and kinetic studies. Journal of CO2 Utilization, 2017, 21, 459-466.	6.8	12
64	A joint MD/QM study on the possibility of alkaloids detection by cucurbiturils and graphene oxide-cucurbituril composites. Journal of Molecular Liquids, 2018, 272, 963-972.	4.9	12
65	DFT investigation on the selective complexation of Fe 3+ and Al 3+ with hydroxypyridinones used for treatment of the aluminium and iron overload diseases. Journal of Molecular Graphics and Modelling, 2018, 80, 182-189.	2.4	11
66	Evaluation of Nâ€”H...S and Nâ€”H...Ïâ€ interactions inO,Oâ€²-diethylN-(2,4,6-trimethylphenyl)thiophosphate: a combination of X-ray crystallographic and theoretical studies. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 847-855.	0.5	11
67	RNA aptasensor based on gold nanoparticles for selective detection of neomycin B, molecular approach. Journal of the Iranian Chemical Society, 2019, 16, 2389-2400.	2.2	11
68	The investigation of the G-quadruplex aptamer selectivity to Pb²⁺ ion: a joint molecular dynamics simulation and density functional theory study. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3659-3675.	3.5	11
69	A combined molecular dynamics and quantum mechanics study on the interaction of Fe3+ and human serum albumin relevant to iron overload disease. Journal of Molecular Liquids, 2020, 317, 113933.	4.9	11
70	Theoretical investigation of the chemoselectivity and synchronously pyrazole ring formation mechanism from ethoxymethylenemalononitrile and hydrazine hydrate in the gas and solvent phases: DFT, meta-GGA studies and NBO analysis. RSC Advances, 2014, 4, 43485-43495.	3.6	10
71	N-Ethylcarbazole-doped fullerene as a potential candidate for hydrogen storage, a kinetics approach. RSC Advances, 2015, 5, 49159-49167.	3.6	10
72	A comprehensive study of the solvent effects on the cycloaddition reaction of diethyl azodicarboxylate and ethyl vinyl ether: Efficient implementation of QM and TD-DFT study. International Journal of Quantum Chemistry, 2015, 115, 381-388.	2.0	10

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73	Pâ€doped <scp>gâ€C₃N₄</scp> as an efficient photocatalyst for <scp>CO₂</scp> conversion into valueâ€added materials: a joint experimental and theoretical study. International Journal of Quantum Chemistry, 2020, 120, e26388.	2.0	10
74	The effects of amino acid sequence and solvent polarity on the self-assembling of cyclic peptide nanotubes and molecular channel formation inside the lipid bilayer. Journal of Molecular Liquids, 2020, 314, 113660.	4.9	10
75	DFT Calculations on Retro-Ene Reactions Part I: Allyl n-Butyl Sulfide Pyrolysis in the Gas Phase. Journal of Chemical Research, 2004, 2004, 585-588.	1.3	9
76	DFT investigation on the selective complexation of ionic liquids based on Î±-amino acid anion and N7,N9-dimethyladeninium cation with CO₂. RSC Advances, 2016, 6, 85924-85932.	3.6	9
77	Computational Kinetic Modeling of the Catalytic Cycle of Glutathione Peroxidase Nanomimic: Effect of Nucleophilicity of Thiols on the Catalytic Activity. Journal of Physical Chemistry A, 2018, 122, 364-374.	2.5	9
78	Solvent Effects on Intra-/Intermolecular Charge Transfer in Indoloquinoxaline-Based Dyes. Journal of Physical Chemistry A, 2019, 123, 2831-2842.	2.5	9
79	Theoretical study on the absorption of carbon dioxide by DBU-based ionic liquids. Physical Chemistry Chemical Physics, 2020, 22, 20050-20060.	2.8	9
80	Computational modeling of the kinetics and mechanism of telluriumâ€based glutathione peroxidase mimic. International Journal of Quantum Chemistry, 2020, 120, e26201.	2.0	9
81	Temperature and molecular crowding effects on the sensitivity of T30695 aptamer toward Pb²⁺ion: a joint molecular dynamics simulation and experimental study. Molecular Simulation, 2020, 46, 592-603.	2.0	9
82	DFT calculations on the retro-ene reactions, part II: allyl n-propyl sulfide pyrolysis in the gas phase. Computational and Theoretical Chemistry, 2004, 686, 37-42.	1.5	8
83	A joint experimental and computational study on the kinetic and mechanism of diallyl disulfide pyrolysis in the gas phase. Chemical Physics, 2004, 301, 45-51.	1.9	8
84	Computational Modeling of the Catalytic Cycle of Glutathione Peroxidase Nanomimic. Journal of Physical Chemistry A, 2016, 120, 10108-10115.	2.5	8
85	Fischerâ€“Tropsch synthesis over a novel cobalt catalyst supported on UiO-66. Journal of the Iranian Chemical Society, 2021, 18, 1043-1050.	2.2	8
86	Thermal decomposition mechanisms of the ionic liquids based on Î±-amino acid anion and N7,N9-dimethyladeninium cation: Quantum chemistry approach. Journal of Molecular Liquids, 2015, 209, 779-784.	4.9	7
87	Understanding the role of noncovalent interactions on the rate of some Dielsâ€Alder reactions in different solvents. International Journal of Quantum Chemistry, 2019, 119, e25878.	2.0	7
88	Molecular electrostatic potential at nuclear position as a new concept in evaluation of the substitution effects of intramolecular B/N frustrated Lewis pairs in H 2 splitting and CO 2 reduction. International Journal of Quantum Chemistry, 2020, 120, e26416.	2.0	7
89	Molecular engineering of triphenylamineâ€based metalâ€free organic dyes for dyeâ€sensitized solar cells. International Journal of Quantum Chemistry, 2021, 121, e26620.	2.0	7
90	The influence of hydrophobic amino acid side groups on the acidity of the aromatic imidazole ring of histidine: A theoretical study. International Journal of Quantum Chemistry, 2012, 112, 2675-2680.	2.0	6

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91	Quantum chemistry study on the mechanism of oxidation of cysteine to cystine using hydrogen peroxide. Phosphorus, Sulfur and Silicon and the Related Elements, 2015, 190, 1680-1691.	1.6	6
92	Understanding the thermodynamic and kinetic performances of the substituted phosphorus ylides as a new class of compounds in carbon dioxide activation. Energy, 2018, 145, 329-337.	8.8	6
93	MD/QM modeling of the modified gold nanoparticles and investigation of their sensing ability for selective detection of melamine. Journal of Molecular Liquids, 2019, 284, 454-461.	4.9	6
94	Effect of electron donor and acceptor on the photovoltaic properties of organic dyes for efficient dye-sensitized solar cells. Physica B: Condensed Matter, 2021, 609, 412815.	2.7	6
95	Theoretical prediction of voltage-current behavior and other photovoltaic properties of natural flavonoid-based solar cells. Solar Energy, 2021, 228, 89-99.	6.1	6
96	Thermal decomposition mechanisms of some amino acid ionic liquids: Molecular approach. Journal of Molecular Liquids, 2020, 302, 112505.	4.9	6
97	Thermal decomposition of amino acid ionic liquids: Mechanism insight. Journal of Molecular Liquids, 2022, 349, 118486.	4.9	6
98	ZIF-8 metal-organic framework conjugated to pristine and doped B12N12 nanoclusters as a new hybrid nanomaterial for detection of amphetamine. Inorganic Chemistry Communication, 2022, 135, 109119.	3.9	6
99	A theoretical approach on the ability of functionalized gold nanoparticles for detection of Cd2+. Scientific Reports, 2021, 11, 23422.	3.3	6
100	Ionic liquids based on Î±-amino acids; a structural insights into [dMA][AA] and computational evaluation of the hydrogen bonds. Journal of Molecular Liquids, 2014, 200, 439-447.	4.9	5
101	Computational kinetic modeling of the selenol catalytic activity as the glutathione peroxidase nanomimic. Journal of Theoretical Biology, 2016, 409, 108-114.	1.7	5
102	Theoretical investigation of the thermal decomposition of imidazolium ionic liquids with different halides ions. Journal of Molecular Liquids, 2016, 224, 460-465.	4.9	5
103	A theoretical study on the electronic structures and equilibrium constants evaluation of Deferasirox iron complexes. Computational Biology and Chemistry, 2016, 64, 99-106.	2.3	5
104	The Molecular Adsorption of Carbon Monoxide on Cobalt Surfaces: A Dft Study. Progress in Reaction Kinetics and Mechanism, 2017, 42, 89-98.	2.1	5
105	Antioxidant activity of selenenamide-based mimic as a function of the aromatic thiols nucleophilicity, a DFT-SAPE model. Computational Biology and Chemistry, 2018, 75, 213-221.	2.3	5
106	Theoretical study on alkaloid encapsulating via monohydroxy-cucurbit[n]uril (nâ€¯=â€¯8,10)/graphene oxide composite. Journal of Molecular Liquids, 2019, 288, 111085.	4.9	5
107	Drugâ€“DNA interaction, a joint DFT-D3/MD study on safranal as an anticancer and DNA nanostructure model. Canadian Journal of Chemistry, 2019, 97, 120-130.	1.1	5
108	Insight into incident photon to current conversion efficiency in chlorophylls. International Journal of Quantum Chemistry, 2021, 121, e26483.	2.0	5

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109	Photovoltaic and spectroscopic properties of bacteriochlorin-based photosensitizer: molecular approach. Research on Chemical Intermediates, 2021, 47, 1071-1085.	2.7	5
110	QM/MD study on the ability of phosphorene for selective detection of amino acids. Journal of Molecular Liquids, 2021, 336, 116865.	4.9	5
111	A Computational Study of the Kinetics and Mechanism of the Gas Phase Pyrolysis of Allyl Methyl Amine. Progress in Reaction Kinetics and Mechanism, 2011, 36, 63-72.	2.1	4
112	Structure-Activity Relationship for Fe(III)-Salen-Like Complexes as Potent Anticancer Agents. Scientific World Journal, The, 2014, 2014, 1-10.	2.1	4
113	A facile access to highly functionalized triphenylphosphoranylidene succinimides through a three-component reaction and DFT investigation of the reaction mechanism. RSC Advances, 2014, 4, 37900.	3.6	4
114	Density functional theory study of the regioâ€•and stereoselectivity of 1,3-dipolar cycloaddition reactions between 2-ethylthio-4-phenyl-1-azetin and some substituted nitrile oxides. Structural Chemistry, 2016, 27, 1041-1047.	2.0	4
115	Surface Decomposition of Dimethyl Methylphosphonate on SnO₂ Nanoparticles: Role of Nanoparticle Size. Progress in Reaction Kinetics and Mechanism, 2017, 42, 99-110.	2.1	4
116	Kinetics and mechanism of 2-pyridylacetic acid pyrolysis in the gas phase: A joint experimental and theoretical study. Chemical Physics, 2006, 330, 394-400.	1.9	3
117	Gas Phase Pyrolysis Reaction of 1-pyrazoline: A Theoretical Kinetic Study. Progress in Reaction Kinetics and Mechanism, 2012, 37, 423-435.	2.1	3
118	Quantum chemical aspects of solvent effects on the Dielsâ€“Alder reaction of 2,3-dimethyl-1,3-butadiene and diethyl azodicarboxylate. Progress in Reaction Kinetics and Mechanism, 2016, 41, 224-234.	2.1	3
119	A DFT study of solvent effects on the kinetics and mechanism of the [3,3] hetero-Cope rearrangement of 1-butene thiobenzoate. Progress in Reaction Kinetics and Mechanism, 2016, 41, 153-158.	2.1	3
120	A molecular approach on the ability of functionalized gold nanoparticles for selective sensing of Hg2+. Journal of Molecular Liquids, 2019, 292, 111461.	4.9	3
121	The first coordination polymers with an [O]₂[N]P(S)-Hg segment: a combined experimental, theoretical and database study. Dalton Transactions, 2019, 48, 17908-17918.	3.3	3
122	Threonine stabilizerâ€controlled wellâ€dispersed small palladium nanoparticles on modified magnetic nanocatalyst for Heck crossâ€coupling process in water. Applied Organometallic Chemistry, 2019, 33, e4645.	3.5	3
123	Optoelectronic properties and energy conversion of organic dye-based solar cells: Molecular approach. Optik, 2020, 203, 163972.	2.9	3
124	The reactivity enhancement in Dielsâ€“Alder cycloaddition of 1,3-diene by cation encapsulation to C60: a computational insight. Structural Chemistry, 2020, 31, 1821-1829.	2.0	3
125	Theoretical designing and understanding of the performances of Bï£¿H bridged organocatalysts by Ïâ€conjugated molecules in CO 2 hydroboration. International Journal of Quantum Chemistry, 2021, 121, e26512.	2.0	3
126	Insight into the semiconducting performance of tetraphenyldipyranylidene derivatives in organic fieldâ€effect transistors. International Journal of Quantum Chemistry, 2021, 121, qua26678.	2.0	3

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127	Substituent effects and mechanism studies in <scp>CO₂</scp> transformation to benzoxazinone derivatives as worthwhile Nâ€containing heterocycles: Insight from <scp>Density functional theory</scp>. International Journal of Quantum Chemistry, 2021, 121, e26784.	2.0	3
128	Substitution effect on electronic and optical properties of Tetraphenyldipyranylidene; A theoretical study. Journal of Physics and Chemistry of Solids, 2022, 162, 110504.	4.0	3
129	Quantum chemistry calculations of S, P, and O-doping effect on the photocatalytic molecular descriptors of g-C3N4 quantum dots. Journal of the Iranian Chemical Society, 2022, 19, 3513-3528.	2.2	3
130	Cyclic Nanostructures of Tungsten OxideWO3nâ€‰â€‰(n=2â€“6)asNOxGas Sensor: A Theoretical Study. International Journal of Analytical Chemistry, 2014, 2014, 1-6.	1.0	2
131	Different Aspects of Single Wall Carbon Nanotube Functionalization by Aniline Adsorption; Quantum Mechanics/Molecular Mechanics Study. Journal of Nano Research, 2015, 32, 1-16.	0.8	2
132	NCI concept as a powerful tool to investigate the origin of Dielsâ€“Alder reaction accelerating inside the self-assembled softball nanoreactor. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 85, 237-246.	1.6	2
133	Theoretical evaluation of symmetrical Î±,Î±â€²,Î´,Î´â€²-tetramethyl cucurbit[6]uril for haloalkane 1-(3-chlorophenyl)-4-(3-chloropropyl)-piperazinium and chloroform encapsulation. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2018, 92, 103-114.	1.6	2
134	Theoretical study on ionic liquids based on DBUH + : Molecular engineering and hydrogen bond evaluation. International Journal of Quantum Chemistry, 2019, 119, e25966.	2.0	2
135	Exploring the interaction of amino acid-based ionic liquids in water and organic solvents: Insight from MD simulations and QM calculations. Journal of Molecular Liquids, 2021, 327, 114867.	4.9	2
136	Solvent effect on the efficiency of triphenylamine-based dye-sensitized solar cells, molecular approach. Chemical Physics, 2022, 561, 111594.	1.9	2
137	A Theoretical Study of the Mechanism and Kinetics of the Thermal Decomposition of Carbamoyl Azide. Progress in Reaction Kinetics and Mechanism, 2013, 38, 305-315.	2.1	1
138	N-Phenyl-1-methyl-6-methylenecyclohexa-2,4-dienylmethanimine retro cheletropic-ene reaction, a theoretical kinetic study. Progress in Reaction Kinetics and Mechanism, 2013, 38, 408-416.	2.1	1
139	Kinetics and mechanism of diallyl sulfoxide pyrolysis; a combined theoretical and experimental study in the gas phase. RSC Advances, 2014, 4, 62809-62816.	3.6	1
140	Computational study on the mechanism of N-phenylimine derivativesâ€™ pyrolysis reaction in the gas phase. Journal of the Iranian Chemical Society, 2014, 11, 399-406.	2.2	1
141	Implicit and explicit solvent effects on the selectivity of the cycloaddition reaction of cyclopentadiene and methyl acrylate; a theoretical study. Progress in Reaction Kinetics and Mechanism, 2015, 40, 303-312.	2.1	1
142	A Qm/Mm Study of No Oxidation on the Nanocrystalline Surface of Tungsten Oxide. Progress in Reaction Kinetics and Mechanism, 2015, 40, 69-76.	2.1	1
143	A Combined Quantum Mechanics and Molecular Mechanics Study on Nitrogen Oxide Adsorption/Dissociation on a Tungsten Oxide Surface. Progress in Reaction Kinetics and Mechanism, 2015, 40, 128-142.	2.1	1
144	Stereoelectronic Effects: A Powerful Concept in Explaining Kinetic and Thermodynamic Aspects of Retro Cheletropic Reactions. Journal of Chemical Research, 2015, 39, 635-639.	1.3	1

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145	Theoretical Evaluation of the Efficiency of Novel Frustrated Lewis Pairs in the cis-Hydrogenation Reaction of Dimethylacetylene. Progress in Reaction Kinetics and Mechanism, 2017, 42, 372-383.	2.1	1
146	Direct C2-arylation of quinoline N-oxides by boronic esters; a molecular approach on the efficient metal-free method in Câ€“C cross-coupling reactions. Research on Chemical Intermediates, 2018, 44, 657-673.	2.7	1
147	Computational modeling of the kinetics and mechanism of the new generation of glutathione peroxidase nanomimic: selenosubtilisin and tellurosubtilisin. Journal of the Iranian Chemical Society, 2020, 17, 2119-2131.	2.2	1
148	The effect of the central metal ion on photovoltaic properties of bacteriochlorin derivatives. Materials Today Communications, 2021, 27, 102367.	1.9	1
149	Theoretical Approaches to CO2 Transformations. Advances in Science, Technology and Innovation, 2022, , 153-220.	0.4	1
150	Chemical wave studies in the bromateâ€“pyrocatechol beads system. International Journal of Chemical Kinetics, 2011, 43, 198-203.	1.6	0
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