

# Mohammad Izadyar

## List of Publications by Year in descending order

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154  
papers

1,744  
citations

430442

18  
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476904

29  
g-index

162  
all docs

162  
docs citations

162  
times ranked

1657  
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. <i>Biosensors and Bioelectronics</i> , 2018, 122, 263-283.	5.3	124
2	A simple paper-based aptasensor for ultrasensitive detection of lead (II) ion. <i>Analytica Chimica Acta</i> , 2019, 1071, 70-77.	2.6	61
3	Hydrogen storage by N-ethylcarbazol as a new liquid organic hydrogen carrier: A DFT study on the mechanism. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 5797-5806.	3.8	50
4	Theoretical Design of Functionalized Gold Nanoparticles as Antiviral Agents against Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2). <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 10284-10289.	2.1	45
5	Size-controlled synthesis of SnO <sub>2</sub> nanoparticles using reverse microemulsion method. <i>Solid State Sciences</i> , 2014, 33, 6-11.	1.5	40
6	The role of the electronic structure and solvent in the dye-sensitized solar cells based on Zn-porphyrins: Theoretical study. <i>Energy</i> , 2016, 114, 559-567.	4.5	36
7	Fischer-Tropsch synthesis using zeolitic imidazolate framework (ZIF-7 and ZIF-8)-supported cobalt catalysts. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5747.	1.7	33
8	Dissociative hydrogen adsorption on the cubic cobalt surfaces: A DFT study. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 7064-7071.	3.8	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. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 11382-11391.	1.3	29
10	The investigation of the central metal effects on the porphyrin-based DSSCs performance; molecular approach. <i>Materials Chemistry and Physics</i> , 2017, 196, 142-152.	2.0	28
11	DFT investigation and molecular dynamic simulation on the selective complexation of cis-cyclic nanopptides with alkaline earth metal ions. <i>Sensors and Actuators B: Chemical</i> , 2015, 221, 1120-1129.	4.0	27
12	Recent theoretical progress in the organic/metal-organic sensitizers as the free dyes, dye/TiO <sub>2</sub> and dye/electrolyte systems; Structural modifications and solvent effects on their performance. <i>Renewable and Sustainable Energy Reviews</i> , 2018, 94, 609-655.	8.2	26
13	Efficient synthesis of novel spiro[indole-3,6 <sup>2</sup> -pyrano[2,3-d][1,3]thiazolo[3,2-a]pyrimidine derivatives through an organobase-catalyzed, three-component reaction. <i>Tetrahedron</i> , 2015, 71, 2458-2462.	1.0	23
14	Anchoring Group and ĩ-Spacer Effects on the Dynamics and Kinetics of the Photovoltaic Processes in the Quinoxaline-Based Organic Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2018, 122, 23968-23977.	1.5	22
15	Evaluation and understanding the performances of various derivatives of carbonyl-stabilized phosphonium ylides in CO <sub>2</sub> transformation to cyclic carbonates. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 223-237.	1.3	21
16	Recent advances in computational methods for biosensor design. <i>Biotechnology and Bioengineering</i> , 2021, 118, 555-578.	1.7	20
17	A Computational Exploration of H <sub>2</sub> S and CO <sub>2</sub> Capture by Ionic Liquids Based on ĩ-Amino Acid Anion and N <sup>7</sup> , N <sup>9</sup> -Dimethyladeninium Cation. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4352-4362.	1.1	19
18	Theoretical design and experimental study on the gold nanoparticles based colorimetric aptasensors for detection of neomycin B. <i>Sensors and Actuators B: Chemical</i> , 2019, 300, 126947.	4.0	19

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19	Mechanistic double ASF product distribution study of Fischer–Tropsch synthesis on precipitated iron catalyst. <i>Journal of Natural Gas Science and Engineering</i> , 2013, 15, 53-58.	2.1	18
20	Theoretical design of the cyclic lipopeptide nanotube as a molecular channel in the lipid bilayer, molecular dynamics and quantum mechanics approach. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 25536-25549.	1.3	17
21	Solvent and spin state effects on molecular structure, IR spectra, binding energies and quantum chemical reactivity indices of deferiprone–ferric complex: DFT study. <i>Polyhedron</i> , 2016, 117, 623-627.	1.0	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. <i>Energy</i> , 2017, 134, 493-503.	4.5	17
23	Theoretical evaluation of N-alkylcarbazoles potential in hydrogen release. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 9966-9977.	3.8	17
24	Detailed kinetics of Fischer–Tropsch synthesis on a precipitated iron catalyst. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2014, 111, 29-44.	0.8	16
25	A DFT study on the complex formation between desferrithiocin and metal ions (Mg <sup>2+</sup> , Al <sup>3+</sup> , Ca <sup>2+</sup> ,) Tj ETQq1 1 0.784314 rgBT /Overlo	1.1	16
26	DFT study on the selective complexation of B <sub>12</sub> nanocage with alkali metal ions. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2018, 193, 178-184.	0.8	16
27	Theoretical design and experimental study of new aptamers with the improved target-affinity: New insights into the Pb <sup>2+</sup> -specific aptamers as a case study. <i>Journal of Molecular Liquids</i> , 2019, 289, 111159.	2.3	16
28	Gas-phase kinetics and mechanism of diallyl sulfide thermal decomposition. <i>Journal of Physical Organic Chemistry</i> , 2003, 16, 153-157.	0.9	15
29	Combination of X-ray crystallography and theoretical study to evaluate the effect of NH <sup>+</sup> OP versus NH <sup>+</sup> OC hydrogen bonds on the NH stretching frequencies. <i>Journal of Molecular Structure</i> , 2013, 1034, 354-362.	1.8	15
30	Quantum Chemistry Aspects of the Solvent Effects on 3,4-Dimethyl-2,5-dihydrothiophen-1,1-dioxide Pyrolysis Reaction. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2427-2433.	1.1	15
31	The effect of glycosylation on the transferrin structure: A molecular dynamic simulation analysis. <i>Journal of Theoretical Biology</i> , 2016, 404, 73-81.	0.8	15
32	Effects of synergistic and non-synergistic anions on the iron binding site from serum transferrin: A molecular dynamic simulation analysis. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 78, 176-186.	1.3	15
33	Modeling of the Functionalized Gold Nanoparticle Aggregation in the Presence of Dopamine: A Joint MD/QM Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 26130-26141.	1.5	15
34	A DFT study on the metal ion selectivity of deferiprone complexes. <i>Computational Biology and Chemistry</i> , 2020, 86, 107267.	1.1	15
35	First-principles study of the binding affinity of monolayer BC <sub>6</sub> N nanosheet: Implications for drug delivery. <i>Materials Chemistry and Physics</i> , 2022, 276, 125375.	2.0	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. <i>Computational and Theoretical Chemistry</i> , 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. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 666-674.	1.0	14
38	A quantum chemistry study on the performance of porphyrin-based solar cell sensitizers; Zinc and anchor group position effects. <i>Molecular Physics</i> , 2015, 113, 3815-3825.	0.8	14
39	The origin of regio- and stereoselectivity in the 1,3-dipolar cycloaddition of nitrile oxides with C <sub>1</sub> -substituted 7-oxabenzonorbornadienes, a DFT study. <i>RSC Advances</i> , 2015, 5, 38489-38498.	1.7	14
40	Borohydride salts as high efficiency reducing reagents for carbon dioxide transformation to methanol: Theoretical approach. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 11131-11140.	3.8	14
41	Understanding the mechanism, thermodynamic and kinetic features of the Kukhtin-Ramirez reaction in carbamate synthesis from carbon dioxide. <i>RSC Advances</i> , 2017, 7, 1701-1710.	1.7	14
42	Highly Dispersed Palladium Nanoparticle-Loaded Magnetic Catalyst (FeS@EP-AG-Pd) for Suzuki Reaction in Water. <i>Catalysis Letters</i> , 2017, 147, 1162-1171.	1.4	14
43	Molecular engineering of the organometallic perovskites/HTMs in the PSCs: Photovoltaic behavior and energy conversion. <i>Solar Energy Materials and Solar Cells</i> , 2018, 180, 46-58.	3.0	14
44	Molecular dynamic simulation and DFT study on the Drug-DNA interaction; Crocetin as an anti-cancer and DNA nanostructure model. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 1063-1074.	2.0	14
45	Computational modeling of the photovoltaic activities in EABX3 (EA <sup>-</sup> =ethylammonium, B <sup>-</sup> =Pb, Sn, Ge.) <i>TJFTQq1</i> 1.0.78431	1.4	14
46	Advances in molecular engineering of organic-inorganic/inorganic halide perovskites: Photochemical properties behind the energy conversion ability. <i>Solar Energy</i> , 2019, 194, 51-60.	2.9	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. <i>Applied Physics Letters</i> , 2019, 115, .	1.5	14
48	Substituent effects on the gas phase reactivity of alkyl allyl sulfides, a theoretical study. <i>Computational and Theoretical Chemistry</i> , 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. <i>Tetrahedron Letters</i> , 2014, 55, 333-337.	0.7	13
50	Particle size effects in Fischer-Tropsch synthesis by Co catalyst supported on carbon nanotubes. <i>Chinese Journal of Catalysis</i> , 2015, 36, 1372-1378.	6.9	13
51	Improvement in charge transfer dynamic of the porphyrin-based solar cells in water: A theoretical study. <i>Journal of Renewable and Sustainable Energy</i> , 2017, 9, .	0.8	13
52	Sensing Ability of Hybrid Cyclic Nanopeptides Based on Thiourea Cryptands for Different Ions, A Joint DFT-D3/MD Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 244-255.	1.1	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. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 71, 28-39.	1.3	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. <i>Structural Chemistry</i> , 2017, 28, 675-686.	1.0	13

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55	Proton sponge as a new efficient catalyst for carbon dioxide transformation to methanol: Theoretical approach. <i>Fuel</i> , 2018, 221, 491-500.	3.4	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. <i>Journal of Molecular Structure</i> , 2018, 1166, 448-455.	1.8	13
57	A joint QM/MD study on $\hat{I}^{\pm}$ , $\hat{I}^2$ - and $\hat{I}^3$ -cyclodextrins in selective complexation with cathinone. <i>Supramolecular Chemistry</i> , 2018, 30, 687-696.	1.5	13
58	Carbon Dioxide Absorption by the Imidazolium-based Amino Acid Ionic Liquids, Kinetics, and Mechanism Approach. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5721-5729.	1.1	13
59	A combined MD/QM study on the sensing mechanism of Pb <sup>2+</sup> by glutathione functionalized gold nanoparticles. <i>Journal of Molecular Liquids</i> , 2019, 280, 120-127.	2.3	13
60	Photovoltaic properties of the flavonoid-based photosensitizers: Molecular-scale perspective on the natural dye solar cells. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26171.	1.0	13
61	A molecular dynamic study on the ability of phosphorene for designing new sensor for SARS-CoV-2 detection. <i>Journal of Molecular Liquids</i> , 2022, 345, 117852.	2.3	13
62	The role of solvent and structure in the kinetics of the excitons in porphyrin-based hybrid solar cells. <i>Solar Energy</i> , 2017, 146, 368-378.	2.9	12
63	Phosphorus ylides as a new class of compounds in CO <sub>2</sub> activation: Thermodynamic and kinetic studies. <i>Journal of CO<sub>2</sub> Utilization</i> , 2017, 21, 459-466.	3.3	12
64	A joint MD/QM study on the possibility of alkaloids detection by cucurbiturils and graphene oxide-cucurbituril composites. <i>Journal of Molecular Liquids</i> , 2018, 272, 963-972.	2.3	12
65	DFT investigation on the selective complexation of Fe <sup>3+</sup> and Al <sup>3+</sup> with hydroxypyridinones used for treatment of the aluminium and iron overload diseases. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 80, 182-189.	1.3	11
66	Evaluation of Nâ€”H...S and Nâ€”H...Ï€ interactions in <i>O</i> , <i>O</i> -diethyl- <i>N</i> -(2,4,6-trimethylphenyl)thiophosphate: a combination of X-ray crystallographic and theoretical studies. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 847-855.	0.2	11
67	RNA aptasensor based on gold nanoparticles for selective detection of neomycin B, molecular approach. <i>Journal of the Iranian Chemical Society</i> , 2019, 16, 2389-2400.	1.2	11
68	The investigation of the G-quadruplex aptamer selectivity to Pb <sup>2+</sup> ion: a joint molecular dynamics simulation and density functional theory study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 3659-3675.	2.0	11
69	A combined molecular dynamics and quantum mechanics study on the interaction of Fe <sup>3+</sup> and human serum albumin relevant to iron overload disease. <i>Journal of Molecular Liquids</i> , 2020, 317, 113933.	2.3	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. <i>RSC Advances</i> , 2014, 4, 43485-43495.	1.7	10
71	N-Ethylcarbazole-doped fullerene as a potential candidate for hydrogen storage, a kinetics approach. <i>RSC Advances</i> , 2015, 5, 49159-49167.	1.7	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. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 381-388.	1.0	10

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73	P-doped $\text{g-C}_3\text{N}_4$ as an efficient photocatalyst for $\text{CO}_2$ conversion into value-added materials: a joint experimental and theoretical study. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26388.	1.0	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. <i>Journal of Molecular Liquids</i> , 2020, 314, 113660.	2.3	10
75	DFT Calculations on Retro-Ene Reactions Part I: Allyl n-Butyl Sulfide Pyrolysis in the Gas Phase. <i>Journal of Chemical Research</i> , 2004, 2004, 585-588.	0.6	9
76	DFT investigation on the selective complexation of ionic liquids based on $\alpha$ -amino acid anion and N7,N9-dimethyladeninium cation with $\text{CO}_2$ . <i>RSC Advances</i> , 2016, 6, 85924-85932.	1.7	9
77	Computational Kinetic Modeling of the Catalytic Cycle of Glutathione Peroxidase Nanomimic: Effect of Nucleophilicity of Thiols on the Catalytic Activity. <i>Journal of Physical Chemistry A</i> , 2018, 122, 364-374.	1.1	9
78	Solvent Effects on Intra-/Intermolecular Charge Transfer in Indoloquinoline-Based Dyes. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2831-2842.	1.1	9
79	Theoretical study on the absorption of carbon dioxide by DBU-based ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20050-20060.	1.3	9
80	Computational modeling of the kinetics and mechanism of tellurium-based glutathione peroxidase mimic. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26201.	1.0	9
81	Temperature and molecular crowding effects on the sensitivity of T30695 aptamer toward $\text{Pb}^{2+}$ ion: a joint molecular dynamics simulation and experimental study. <i>Molecular Simulation</i> , 2020, 46, 592-603.	0.9	9
82	DFT calculations on the retro-ene reactions, part II: allyl n-propyl sulfide pyrolysis in the gas phase. <i>Computational and Theoretical Chemistry</i> , 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. <i>Chemical Physics</i> , 2004, 301, 45-51.	0.9	8
84	Computational Modeling of the Catalytic Cycle of Glutathione Peroxidase Nanomimic. <i>Journal of Physical Chemistry A</i> , 2016, 120, 10108-10115.	1.1	8
85	Fischer-Tropsch synthesis over a novel cobalt catalyst supported on UiO-66. <i>Journal of the Iranian Chemical Society</i> , 2021, 18, 1043-1050.	1.2	8
86	Thermal decomposition mechanisms of the ionic liquids based on $\alpha$ -amino acid anion and N7,N9-dimethyladeninium cation: Quantum chemistry approach. <i>Journal of Molecular Liquids</i> , 2015, 209, 779-784.	2.3	7
87	Understanding the role of noncovalent interactions on the rate of some Diels-Alder reactions in different solvents. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25878.	1.0	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 $\text{H}_2$ splitting and $\text{CO}_2$ reduction. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26416.	1.0	7
89	Molecular engineering of triphenylamine-based metal-free organic dyes for dye-sensitized solar cells. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26620.	1.0	7
90	The influence of hydrophobic amino acid side groups on the acidity of the aromatic imidazole ring of histidine: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2675-2680.	1.0	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.	0.8	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.	4.5	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.	2.3	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.	1.3	6
95	Theoretical prediction of voltage-current behavior and other photovoltaic properties of natural flavonoid-based solar cells. Solar Energy, 2021, 228, 89-99.	2.9	6
96	Thermal decomposition mechanisms of some amino acid ionic liquids: Molecular approach. Journal of Molecular Liquids, 2020, 302, 112505.	2.3	6
97	Thermal decomposition of amino acid ionic liquids: Mechanism insight. Journal of Molecular Liquids, 2022, 349, 118486.	2.3	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.	1.8	6
99	A theoretical approach on the ability of functionalized gold nanoparticles for detection of Cd <sup>2+</sup> . Scientific Reports, 2021, 11, 23422.	1.6	6
100	Ionic liquids based on $\hat{L}$ -amino acids; a structural insights into [DMA][AA] and computational evaluation of the hydrogen bonds. Journal of Molecular Liquids, 2014, 200, 439-447.	2.3	5
101	Computational kinetic modeling of the selenol catalytic activity as the glutathione peroxidase nanomimic. Journal of Theoretical Biology, 2016, 409, 108-114.	0.8	5
102	Theoretical investigation of the thermal decomposition of imidazolium ionic liquids with different halides ions. Journal of Molecular Liquids, 2016, 224, 460-465.	2.3	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.	1.1	5
104	The Molecular Adsorption of Carbon Monoxide on Cobalt Surfaces: A Dft Study. Progress in Reaction Kinetics and Mechanism, 2017, 42, 89-98.	1.1	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.	1.1	5
106	Theoretical study on alkaloid encapsulating via monohydroxy-cucurbit[n]uril (n=8,10)/graphene oxide composite. Journal of Molecular Liquids, 2019, 288, 111085.	2.3	5
107	Drug-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.	0.6	5
108	Insight into incident photon to current conversion efficiency in chlorophylls. International Journal of Quantum Chemistry, 2021, 121, e26483.	1.0	5

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109	Photovoltaic and spectroscopic properties of bacteriochlorin-based photosensitizer: molecular approach. <i>Research on Chemical Intermediates</i> , 2021, 47, 1071-1085.	1.3	5
110	QM/MD study on the ability of phosphorene for selective detection of amino acids. <i>Journal of Molecular Liquids</i> , 2021, 336, 116865.	2.3	5
111	A Computational Study of the Kinetics and Mechanism of the Gas Phase Pyrolysis of Allyl Methyl Amine. <i>Progress in Reaction Kinetics and Mechanism</i> , 2011, 36, 63-72.	1.1	4
112	Structure-Activity Relationship for Fe(III)-Salen-Like Complexes as Potent Anticancer Agents. <i>Scientific World Journal</i> , The, 2014, 2014, 1-10.	0.8	4
113	A facile access to highly functionalized triphenylphosphoranylidene succinimides through a three-component reaction and DFT investigation of the reaction mechanism. <i>RSC Advances</i> , 2014, 4, 37900.	1.7	4
114	Density functional theory study of the regio- and stereoselectivity of 1,3-dipolar cycloaddition reactions between 2-ethylthio-4-phenyl-1-azetidin and some substituted nitrile oxides. <i>Structural Chemistry</i> , 2016, 27, 1041-1047.	1.0	4
115	Surface Decomposition of Dimethyl Methylphosphonate on SnO <sub>2</sub> Nanoparticles: Role of Nanoparticle Size. <i>Progress in Reaction Kinetics and Mechanism</i> , 2017, 42, 99-110.	1.1	4
116	Kinetics and mechanism of 2-pyridylacetic acid pyrolysis in the gas phase: A joint experimental and theoretical study. <i>Chemical Physics</i> , 2006, 330, 394-400.	0.9	3
117	Gas Phase Pyrolysis Reaction of 1-pyrazoline: A Theoretical Kinetic Study. <i>Progress in Reaction Kinetics and Mechanism</i> , 2012, 37, 423-435.	1.1	3
118	Quantum chemical aspects of solvent effects on the Diels-Alder reaction of 2,3-dimethyl-1,3-butadiene and diethyl azodicarboxylate. <i>Progress in Reaction Kinetics and Mechanism</i> , 2016, 41, 224-234.	1.1	3
119	A DFT study of solvent effects on the kinetics and mechanism of the [3,3] hetero-Cope rearrangement of 1-butene thiobenzoate. <i>Progress in Reaction Kinetics and Mechanism</i> , 2016, 41, 153-158.	1.1	3
120	A molecular approach on the ability of functionalized gold nanoparticles for selective sensing of Hg <sup>2+</sup> . <i>Journal of Molecular Liquids</i> , 2019, 292, 111461.	2.3	3
121	The first coordination polymers with an [O] <sub>2</sub> [N]P(S)-Hg segment: a combined experimental, theoretical and database study. <i>Dalton Transactions</i> , 2019, 48, 17908-17918.	1.6	3
122	Threonine stabilizer-controlled well-dispersed small palladium nanoparticles on modified magnetic nanocatalyst for Heck cross-coupling process in water. <i>Applied Organometallic Chemistry</i> , 2019, 33, e4645.	1.7	3
123	Optoelectronic properties and energy conversion of organic dye-based solar cells: Molecular approach. <i>Optik</i> , 2020, 203, 163972.	1.4	3
124	The reactivity enhancement in Diels-Alder cycloaddition of 1,3-diene by cation encapsulation to C <sub>60</sub> : a computational insight. <i>Structural Chemistry</i> , 2020, 31, 1821-1829.	1.0	3
125	Theoretical designing and understanding of the performances of Bi <sub>2</sub> H bridged organocatalysts by $\pi$ -conjugated molecules in CO <sub>2</sub> hydroboration. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26512.	1.0	3
126	Insight into the semiconducting performance of tetraphenyldipyranlylidene derivatives in organic field-effect transistors. <i>International Journal of Quantum Chemistry</i> , 2021, 121, qua26678.	1.0	3

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127	Substituent effects and mechanism studies in $\text{CO}_2$ transformation to benzoxazinone derivatives as worthwhile $\text{N}$ -containing heterocycles: Insight from Density functional theory. International Journal of Quantum Chemistry, 2021, 121, e26784.	1.0	3
128	Substitution effect on electronic and optical properties of Tetraphenyldipyranilidene; A theoretical study. Journal of Physics and Chemistry of Solids, 2022, 162, 110504.	1.9	3
129	Quantum chemistry calculations of S, P, and O-doping effect on the photocatalytic molecular descriptors of g-C <sub>3</sub> N <sub>4</sub> quantum dots. Journal of the Iranian Chemical Society, 2022, 19, 3513-3528.	1.2	3
130	Cyclic Nanostructures of Tungsten Oxide $\text{WO}_3$ ( $n=2-6$ ) as $\text{NO}_x$ Gas Sensor: A Theoretical Study. International Journal of Analytical Chemistry, 2014, 2014, 1-6.	0.4	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 Diels-Alder reaction accelerating inside the self-assembled softball nanoreactor. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 85, 237-246.	0.9	2
133	Theoretical evaluation of symmetrical $\beta$ -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.	0.9	2
134	Theoretical study on ionic liquids based on DBUH + : Molecular engineering and hydrogen bond evaluation. International Journal of Quantum Chemistry, 2019, 119, e25966.	1.0	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.	2.3	2
136	Solvent effect on the efficiency of triphenylamine-based dye-sensitized solar cells, molecular approach. Chemical Physics, 2022, 561, 111594.	0.9	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.	1.1	1
138	<i>N</i> -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.	1.1	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.	1.7	1
140	Computational study on the mechanism of <i>N</i> -phenylimine derivatives pyrolysis reaction in the gas phase. Journal of the Iranian Chemical Society, 2014, 11, 399-406.	1.2	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.	1.1	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.	1.1	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.	1.1	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.	0.6	1

#	ARTICLE	IF	CITATIONS
145	Theoretical Evaluation of the Efficiency of Novel Frustrated Lewis Pairs in the <i>cis</i> -Hydrogenation Reaction of Dimethylacetylene. <i>Progress in Reaction Kinetics and Mechanism</i> , 2017, 42, 372-383.	1.1	1
146	Direct C2-arylation of quinoline N-oxides by boronic esters; a molecular approach on the efficient metal-free method in C-C cross-coupling reactions. <i>Research on Chemical Intermediates</i> , 2018, 44, 657-673.	1.3	1
147	Computational modeling of the kinetics and mechanism of the new generation of glutathione peroxidase nanomimic: selenosubtilisin and tellurosutilisin. <i>Journal of the Iranian Chemical Society</i> , 2020, 17, 2119-2131.	1.2	1
148	The effect of the central metal ion on photovoltaic properties of bacteriochlorin derivatives. <i>Materials Today Communications</i> , 2021, 27, 102367.	0.9	1
149	Theoretical Approaches to CO <sub>2</sub> Transformations. <i>Advances in Science, Technology and Innovation</i> , 2022, , 153-220.	0.2	1
150	Chemical wave studies in the bromate-pyrocatechol beads system. <i>International Journal of Chemical Kinetics</i> , 2011, 43, 198-203.	1.0	0
151	First-Principles Calculations on the Kinetics and Mechanism of the Retro-Ene Reaction of Diallyl Amine in the Gas Phase. <i>Progress in Reaction Kinetics and Mechanism</i> , 2012, 37, 193-202.	1.1	0
152	Theoretical study on alkaloid encapsulating via cyclopentano-curbit[ <i>n</i> ]uril ( <i>n</i> = 8, 10)/graphene oxide heterojunction. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26155.	1.0	0
153	QTAIM and NBO Analysis of a New Oxidative Salt of 1,1'-(Ethane-1, 2-diyl) Dipyridinium bisiodate. <i>Oriental Journal of Chemistry</i> , 2014, 30, 785-791.	0.1	0
154	Improvement the energy conversion efficiency of organic dye-based solar cells by pioneer solvents. <i>Molecular Physics</i> , 2022, 120, .	0.8	0