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	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
2	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
3	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
4	Theoretical Approaches to CO2 Transformations. Advances in Science, Technology and Innovation, 2022, , 153-220.	0.4	1
5	Thermal decomposition of amino acid ionic liquids: Mechanism insight. Journal of Molecular Liquids, 2022, 349, 118486.	4.9	6
6	Improvement the energy conversion efficiency of organic dye-based solar cells by pioneer solvents. Molecular Physics, 2022, 120, .	1.7	0
7	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
8	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
9	Solvent effect on the efficiency of triphenylamine-based dye-sensitized solar cells, molecular approach. Chemical Physics, 2022, 561, 111594.	1.9	2
10	Insight into incident photon to current conversion efficiency in chlorophylls. International Journal of Quantum Chemistry, 2021, 121, e26483.	2.0	5
11	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
12	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
13	Theoretical designing and understanding of the performances of Bï£¿H bridged organocatalysts by Ï€â€conjugated molecules in CO 2 hydroboration. International Journal of Quantum Chemistry, 2021, 121, e26512.	2.0	3
14	Recent advances in computational methods for biosensor design. Biotechnology and Bioengineering, 2021, 118, 555-578.	3.3	20
15	Photovoltaic and spectroscopic properties of bacteriochlorin-based photosensitizer: molecular approach. Research on Chemical Intermediates, 2021, 47, 1071-1085.	2.7	5
16	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
17	Insight into the semiconducting performance of tetraphenyldipyranylidene derivatives in organic fieldâ€effect transistors. International Journal of Quantum Chemistry, 2021, 121, qua26678.	2.0	3
18	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

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19	The effect of the central metal ion on photovoltaic properties of bacteriochlorin derivatives. Materials Today Communications, 2021, 27, 102367.	1.9	1
20	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
21	QM/MD study on the ability of phosphorene for selective detection of amino acids. Journal of Molecular Liquids, 2021, 336, 116865.	4.9	5
22	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
23	A theoretical approach on the ability of functionalized gold nanoparticles for detection of Cd2+. Scientific Reports, 2021, 11, 23422.	3.3	6
24	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
25	Theoretical study on alkaloid encapsulating via cyclopentanoâ€cucurbit[n]uril (n =â€‰8, 10)/graphene oxide heterojunction. International Journal of Quantum Chemistry, 2020, 120, e26155.	2.0	0
26	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
27	Optoelectronic properties and energy conversion of organic dye-based solar cells: Molecular approach. Optik, 2020, 203, 163972.	2.9	3
28	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
29	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
30	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
31	Theoretical study on the absorption of carbon dioxide by DBU-based ionic liquids. Physical Chemistry Chemical Physics, 2020, 22, 20050-20060.	2.8	9
32	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
33	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
34	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
35	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
36	Computational modeling of the kinetics and mechanism of telluriumâ€based glutathione peroxidase mimic. International Journal of Quantum Chemistry, 2020, 120, e26201.	2.0	9

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37	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
38	A DFT study on the metal ion selectivity of deferiprone complexes. Computational Biology and Chemistry, 2020, 86, 107267.	2.3	15
39	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
40	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
41	Thermal decomposition mechanisms of some amino acid ionic liquids: Molecular approach. Journal of Molecular Liquids, 2020, 302, 112505.	4.9	6
42	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
43	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
44	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
45	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
46	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
47	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
48	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
49	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
50	A simple paper-based aptasensor for ultrasensitive detection of lead (II) ion. Analytica Chimica Acta, 2019, 1071, 70-77.	5.4	61
51	Solvent Effects on Intra-/Intermolecular Charge Transfer in Indoloquinoxaline-Based Dyes. Journal of Physical Chemistry A, 2019, 123, 2831-2842.	2.5	9
52	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
53	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
54	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

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55	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
56	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
57	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
58	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
59	Proton sponge as a new efficient catalyst for carbon dioxide transformation to methanol: Theoretical approach. Fuel, 2018, 221, 491-500.	6.4	13
60	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
61	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
62	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
63	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
64	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
65	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
66	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
67	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
68	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
69	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
70	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
71	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
72	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

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73	Computational modeling of the photovoltaic activities in EABX3 (EAâ€¯=â€¯ethylammonium, Bâ€¯=â€¯Pb, Sn, Ge,) Tj ETQq1 1 0.784314	3.0	14
74	Evaluation of Nâ€”H...S and Nâ€”H...Ï€ 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
75	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
76	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
77	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
78	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
79	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
80	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
81	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
82	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
83	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
84	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
85	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
86	Theoretical evaluation of N-alkylcarbazoles potential in hydrogen release. International Journal of Hydrogen Energy, 2017, 42, 9966-9977.	7.1	17
87	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
88	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
89	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
90	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

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91	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
92	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
93	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
94	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
95	Computational Modeling of the Catalytic Cycle of Glutathione Peroxidase Nanomimic. Journal of Physical Chemistry A, 2016, 120, 10108-10115.	2.5	8
96	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
97	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
98	Computational kinetic modeling of the selenol catalytic activity as the glutathione peroxidase nanomimic. Journal of Theoretical Biology, 2016, 409, 108-114.	1.7	5
99	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
100	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
101	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
102	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
103	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
104	The effect of glycosylation on the transferrin structure: A molecular dynamic simulation analysis. Journal of Theoretical Biology, 2016, 404, 73-81.	1.7	15
105	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
106	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
107	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
108	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

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109	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
110	N-Ethylcarbazole-doped fullerene as a potential candidate for hydrogen storage, a kinetics approach. RSC Advances, 2015, 5, 49159-49167.	3.6	10
111	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
112	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
113	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
114	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
115	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
116	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
117	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
118	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
119	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
120	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
121	Dissociative hydrogen adsorption on the cubic cobalt surfaces: A DFT study. International Journal of Hydrogen Energy, 2015, 40, 7064-7071.	7.1	30
122	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
123	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
124	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
125	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
126	Structure-Activity Relationship for Fe(III)-Salen-Like Complexes as Potent Anticancer Agents. Scientific World Journal, The, 2014, 2014, 1-10.	2.1	4

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127	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
128	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
129	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
130	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
131	Size-controlled synthesis of SnO2 nanoparticles using reverse microemulsion method. Solid State Sciences, 2014, 33, 6-11.	3.2	40
132	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
133	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
134	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
135	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
136	Detailed kinetics of Fischerâ€“Tropsch synthesis on a precipitated iron catalyst. Reaction Kinetics, Mechanisms and Catalysis, 2014, 111, 29-44.	1.7	16
137	QTAIM and NBO Analysis of a New Oxidative Salt of 1,1/-(Ethane-1, 2-diyl) Dipyridinium bisiodate. Oriental Journal of Chemistry, 2014, 30, 785-791.	0.3	0
138	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
139	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
140	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
141	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
142	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
143	First-Principles Calculations on the Kinetics and Mechanism of the Retro-Ene Reaction of Diallyl Amine in the Gas Phase. Progress in Reaction Kinetics and Mechanism, 2012, 37, 193-202.	2.1	0
144	Gas Phase Pyrolysis Reaction of 1-pyrazoline: A Theoretical Kinetic Study. Progress in Reaction Kinetics and Mechanism, 2012, 37, 423-435.	2.1	3

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145	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
146	Chemical wave studies in the bromateâ€“pyrocatechol beads system. International Journal of Chemical Kinetics, 2011, 43, 198-203.	1.6	0
147	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
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