

# Rita Kakkar

## List of Publications by Year in descending order

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132  
papers

3,066  
citations

257101

24  
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197535

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133  
all docs

133  
docs citations

133  
times ranked

4446  
citing authors

#	ARTICLE	IF	CITATIONS
1	Gallic acid: a versatile antioxidant with promising therapeutic and industrial applications. RSC Advances, 2015, 5, 27540-27557.	1.7	691
2	Isatin and its derivatives: a survey of recent syntheses, reactions, and applications. MedChemComm, 2019, 10, 351-368.	3.5	202
3	Use of metal oxides for the adsorptive removal of toxic organic pollutants. Separation and Purification Technology, 2019, 211, 522-539.	3.9	92
4	Theoretical study of tautomeric structures and fluorescence spectra of Hoechst 33258. Computational and Theoretical Chemistry, 2002, 579, 109-113.	1.5	80
5	An evolving energy solution: Intermediate hydrogen storage. International Journal of Hydrogen Energy, 2018, 43, 12168-12188.	3.8	72
6	Theoretical Study of the Adsorption of Formaldehyde on Magnesium Oxide Nanosurfaces: Size Effects and the Role of Low-Coordinated and Defect Sites. Journal of Physical Chemistry B, 2004, 108, 18140-18148.	1.2	67
7	Hierarchical Porous Magnesium Oxide (Hr-MgO) Microspheres for Adsorption of an Organophosphate Pesticide: Kinetics, Isotherm, Thermodynamics, and DFT Studies. ACS Applied Materials & Interfaces, 2017, 9, 38629-38642.	4.0	66
8	Thiazolidinones: Synthesis, Reactivity, and Their Biological Applications. Journal of Heterocyclic Chemistry, 2019, 56, 1239-1253.	1.4	54
9	Arousing the Reactive Fe Sites in Pyrite (FeS <sub>2</sub> ) via Integration of Electronic Structure Reconfiguration and in Situ Electrochemical Topotactic Transformation for Highly Efficient Oxygen Evolution Reaction. Inorganic Chemistry, 2019, 58, 7615-7627.	1.9	53
10	Conformational behavior of some hydroxamic acids. Organic and Biomolecular Chemistry, 2003, 1, 2200.	1.5	50
11	Recent advances in nano-photocatalysts for organic synthesis. Arabian Journal of Chemistry, 2019, 12, 4550-4578.	2.3	49
12	Graphene-based adsorbents for water remediation by removal of organic pollutants: Theoretical and experimental insights. Chemical Engineering Research and Design, 2020, 153, 21-36.	2.7	48
13	Spectroscopic and molecular modelling studies of binding mechanism of metformin with bovine serum albumin. Journal of Molecular Structure, 2016, 1118, 267-274.	1.8	47
14	Partial molar volumes and adiabatic compressibilities at infinite dilution of aminocarboxylic acids and glycylglycine in water and aqueous solutions of sodium sulphate at (288.15, 298.15 and 308.15)K. Journal of Chemical Thermodynamics, 2006, 38, 1385-1395.	1.0	44
15	Effect of surface passivating ligand on structural and optoelectronic properties of polymer-CdSe quantum dot composites. Journal Physics D: Applied Physics, 2008, 41, 235409.	1.3	44
16	A Chloro-Bridged Heterobimetallic (η <sup>6</sup> -Arene)ruthenium Organotin Complex as an Efficient Topoisomerase II $\alpha$ Inhibitor. Organometallics, 2013, 32, 2546-2551.	1.1	41
17	Magnetically retrievable one-pot fabrication of mesoporous magnesium ferrite (MgFe <sub>2</sub> O <sub>4</sub> ) for the remediation of chlorpyrifos and real pesticide wastewater. Journal of Environmental Chemical Engineering, 2018, 6, 6891-6903.	3.3	38
18	First Principles Density Functional Study of the Adsorption and Dissociation of Carbonyl Compounds on Magnesium Oxide Nanosurfaces. Journal of Physical Chemistry B, 2006, 110, 25941-25949.	1.2	37

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19	Structural aspects of the anti-cancer drug oxaliplatin: A combined theoretical and experimental study. <i>Polyhedron</i> , 2008, 27, 3567-3574.	1.0	33
20	Density functional study of the properties of isomeric aminophenylhydroxamic acids and their copper (II) complexes. <i>Polyhedron</i> , 2006, 25, 759-766.	1.0	32
21	DFT study of structural and electronic properties of gallic acid and its anions in gas phase and in aqueous solution. <i>Structural Chemistry</i> , 2017, 28, 1789-1802.	1.0	31
22	The Curtius rearrangement of some organic azides: A DFT mechanistic study. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1058-1069.	1.0	30
23	Bis-triazolylated-1,4-dihydropyridine - Highly selective hydrophilic fluorescent probe for detection of Fe <sup>3+</sup> . <i>Dyes and Pigments</i> , 2017, 147, 420-428.	2.0	29
24	A DFT study of the structures of pyruvic acid isomers and their decarboxylation. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 886.	1.5	28
25	Adsorption of sarin on MgO nanotubes: Role of doped and defect sites. <i>Journal of Computational Science</i> , 2015, 10, 225-236.	1.5	26
26	<i>In silico</i> studies on potential MCF-7 inhibitors: a combination of pharmacophore and 3D-QSAR modeling, virtual screening, molecular docking, and pharmacokinetic analysis. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017, 35, 1950-1967.	2.0	26
27	DFT study on the adsorption of <i>p</i> -nitrophenol over vacancy and Pt-doped graphene sheets. <i>Computational and Theoretical Chemistry</i> , 2018, 1142, 88-96.	1.1	26
28	Size- and shape-controlled synthesis and properties of colloidal PbSe nanocrystals. <i>Materials Chemistry and Physics</i> , 2009, 113, 107-114.	2.0	24
29	Design, synthesis and biological evaluation of antimalarial activity of new derivatives of 2,4,6-s-triazine. <i>Chemistry Central Journal</i> , 2017, 11, 132.	2.6	24
30	Multifunctional mesoporous curcumin encapsulated iron-phenanthroline nanocluster: A new Anti-HIV agent. <i>Colloids and Surfaces B: Biointerfaces</i> , 2019, 180, 289-297.	2.5	24
31	Tautomeric transformations and reactivity of alloxan. <i>Computational and Theoretical Chemistry</i> , 2012, 986, 14-24.	1.1	23
32	Quantitative Structure Activity Relationship Study of 2,4,6-Trisubstituted- <i>s</i> -Triazine Derivatives as Antimalarial Inhibitors of <i>Plasmodium Falciparum</i> Dihydrofolate Reductase. <i>Chemical Biology and Drug Design</i> , 2011, 77, 57-62.	1.5	22
33	Structures and Stabilities of Alkaline Earth Metal Oxide Nanoclusters: A DFT Study. <i>Journal of Theoretical Chemistry</i> , 2013, 2013, 1-14.	1.5	21
34	Mesoporous rGO@ZnO composite: Facile synthesis and excellent water treatment performance by pesticide adsorption and catalytic oxidative dye degradation. <i>Chemical Engineering Research and Design</i> , 2020, 160, 254-263.	2.7	21
35	Theoretical study of the excited state intramolecular proton transfer in barbituric acid. <i>Computational and Theoretical Chemistry</i> , 2002, 578, 169-175.	1.5	20
36	In Silico study of the active site of <i>Helicobacter pylori</i> urease and its inhibition by hydroxamic acids. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 83, 64-73.	1.3	20

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37	Selective adsorption and separation of toxic cationic dyes using hierarchically porous SDBS modified vaterite microspheres (Hr-SMV). <i>Journal of Physics and Chemistry of Solids</i> , 2020, 146, 109598.	1.9	20
38	Towards understanding the molecular recognition process in Hoechst-DNA complexes. <i>Computational and Theoretical Chemistry</i> , 2002, 584, 37-44.	1.5	19
39	Trans and cis influence in square planar Pt(II) complexes: a density functional study of [PtClX(dms) <sub>2</sub> ] and related complexes. <i>Computational and Theoretical Chemistry</i> , 2004, 679, 149-156.	1.5	19
40	Effect of aqueous solvation on the structures of pyruvic acid isomers and their reactions in solution: a computational study. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 23-29.	0.9	18
41	Role of surface modification of colloidal CdSe quantum dots on the properties of hybrid organic-inorganic nanocomposites. <i>Colloid and Polymer Science</i> , 2010, 288, 841-849.	1.0	18
42	Peanut shell biotemplate to fabricate porous magnetic Co <sub>3</sub> O <sub>4</sub> coral reef and its catalytic properties for p-nitrophenol reduction and oxidative dye degradation. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2020, 604, 125328.	2.3	18
43	Metal ion selectivity of hydroxamates: A density functional study. <i>Computational and Theoretical Chemistry</i> , 2006, 767, 175-184.	1.5	17
44	Controlling the assembly of hydrophobized gold nanoparticles at the air-water interface by varying the interfacial tension. <i>Thin Solid Films</i> , 2010, 519, 1072-1077.	0.8	17
45	Design, Synthesis and Evaluation of 1,2,3-Triazol-4-yl-methyl Tethered 3-Pyrrolylisatins as Potent Anti-Breast Cancer Agents. <i>ChemistrySelect</i> , 2018, 3, 5263-5268.	0.7	17
46	The effect of solvent polarity on the antioxidant potential of echinatin, a retrochalcone, towards various ROS: a DFT thermodynamic study. <i>Free Radical Research</i> , 2020, 54, 777-786.	1.5	17
47	DFT study of adsorption of glyphosate pesticide on Pt-Cu decorated pyridine-like nitrogen-doped graphene. <i>Journal of Nanoparticle Research</i> , 2020, 22, 1.	0.8	17
48	Theoretical study of the effect of radiation on thymine. <i>Computational and Theoretical Chemistry</i> , 2003, 620, 139-147.	1.5	16
49	Hierarchically structured magnesium based oxides: synthesis strategies and applications in organic pollutant remediation. <i>CrystEngComm</i> , 2017, 19, 6913-6926.	1.3	16
50	Adsorption of methyl isocyanate on M <sub>4</sub> (M=Fe, Ni, and Cu) cluster-decorated graphene and vacancy graphene: a DFT-D2 study. <i>Structural Chemistry</i> , 2020, 31, 1983-1997.	1.0	16
51	Theoretical Study of Molecular Recognition by Hoechst 33258 Derivatives. <i>Journal of Biomolecular Structure and Dynamics</i> , 2005, 23, 37-47.	2.0	15
52	An insight into selective and potent inhibition of histone deacetylase 8 through induced-fit docking, pharmacophore modeling and QSAR studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 48-65.	2.0	15
53	Facile synthesis of mesoporous magnesium oxide-graphene oxide composite for efficient and highly selective adsorption of hazardous anionic dyes. <i>Research on Chemical Intermediates</i> , 2020, 46, 2497-2521.	1.3	15
54	C <sub>3</sub> H <sub>4</sub> : Density functional study of interconversion of isomers. <i>International Journal of Quantum Chemistry</i> , 2003, 94, 93-104.	1.0	14

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55	Surface modification of CdSe quantum dots for biosensing applications: Role of ligands. <i>Thin Solid Films</i> , 2010, 519, 1202-1212.	0.8	14
56	Theoretical investigation of the alloxan-dialuric acid redox cycle. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2060-2069.	1.0	14
57	The antioxidant potential of retrochalcones isolated from liquorice root: A comparative DFT study. <i>Phytochemistry</i> , 2021, 192, 112964.	1.4	14
58	C <sub>3</sub> H <sub>4</sub> : density functional (DFT) study of structures and stabilities of isomers. <i>Computational and Theoretical Chemistry</i> , 2002, 617, 141-147.	1.5	13
59	Density functional study of the conformations and intramolecular proton transfer in thiohydroxamic acids. <i>Organic and Biomolecular Chemistry</i> , 2007, 5, 547-557.	1.5	13
60	Theoretical study of the kojic acid structure in gas phase and aqueous solution. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 4318-4329.	1.0	13
61	Theoretical study of the molecular structure and intramolecular proton transfer in benzohydroxamic acid. <i>Computational and Theoretical Chemistry</i> , 2017, 1105, 18-26.	1.1	13
62	Influence of intrinsic and extrinsic factors on the antiradical activity of Gallic acid: a theoretical study. <i>Structural Chemistry</i> , 2018, 29, 359-373.	1.0	12
63	A DFT-D2 study on the adsorption of phosgene derivatives and chloromethyl chloroformate on pristine and Fe <sub>4</sub> -decorated graphene. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 101, 107754.	1.3	12
64	A DFT study of the conformational and electronic properties of echinatin, a retrochalcone, and its anion in the gas phase and aqueous solution. <i>Structural Chemistry</i> , 2020, 31, 2513-2524.	1.0	12
65	Quantum Dots For Diagnosis Of Cancers. <i>Advanced Materials Letters</i> , 2013, 4, 811-822.	0.3	12
66	II-VI core/shell quantum dots and doping with transition metal ions as a means of tuning the magnetoelectronic properties of CdS/ZnS core/shell QDs: A DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 111, 108099.	1.3	12
67	A semiempirical MO study of tautomerism and the electronic structure of barbituric acid. <i>Journal of Chemical Sciences</i> , 1998, 110, 535.	0.7	12
68	Formation of water-soluble and biocompatible TOPO-capped CdSe quantum dots with efficient photoluminescence. <i>Journal of Materials Science: Materials in Medicine</i> , 2009, 20, 123-130.	1.7	11
69	Docking Modes of BB-3497 into the PDF Active Site – A Comparison of the Pure MM and QM/MM Based Docking Strategies. <i>Current Computer-Aided Drug Design</i> , 2015, 10, 315-326.	0.8	11
70	Assessment of molecular binding of Hoechst 33258 analogues into DNA using docking and MM/GBSA approach. <i>Journal of Computational Science</i> , 2015, 10, 166-177.	1.5	11
71	Synthesis and Reactions of Diazoketones. <i>Organic Preparations and Procedures International</i> , 2019, 51, 103-146.	0.6	11
72	Host-guest complexation studies of p-tertbutylcalix[4]arene against ions of interest for radiological decontamination. <i>Inorganica Chimica Acta</i> , 2019, 484, 111-124.	1.2	11

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73	Exploring structural requirements of isoform selective histone deacetylase inhibitors: a comparative <i>in silico</i> study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 502-517.	2.0	11
74	Structure-based virtual screening, free energy of binding and molecular dynamics simulations to propose novel inhibitors of Mtb-MurB oxidoreductase enzyme. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 656-671.	2.0	11
75	Theoretical Study of the Stability of Tautomers and Conformers of Isatin-3-Thiosemicarbazone (IBT). <i>Canadian Chemical Transactions</i> , 0, , 327-342.	0.2	11
76	C3H4: Theoretical study of structures and stabilities of isomers. <i>International Journal of Quantum Chemistry</i> , 1998, 58, 389-398.	1.0	9
77	AM1 study of proton-transfer reactions of barbituric acid. <i>International Journal of Quantum Chemistry</i> , 1999, 74, 327-336.	1.0	9
78	Conformational properties of DNA minor groove binder Hoechst 33258 in gas phase and in aqueous solution. <i>Computational and Theoretical Chemistry</i> , 2017, 1113, 32-41.	1.1	9
79	Synthesis, pharmacological evaluation and molecular docking of pyranopyrazole-linked 1,4-dihydropyridines as potent positive inotropes. <i>Molecular Diversity</i> , 2017, 21, 533-546.	2.1	9
80	Structural, electronic, and reactivity parameters of some triorganotin(IV) carboxylates: a DFT analysis. <i>Structural Chemistry</i> , 2018, 29, 753-763.	1.0	9
81	Identification of novel urease inhibitors: pharmacophore modeling, virtual screening and molecular docking studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 4312-4326.	2.0	9
82	A comparative study of the binding modes of SLC-0111 and its analogues in the hCA II and hCA IX active sites using QM/MM, molecular docking, MM-GBSA and MD approaches. <i>Biophysical Chemistry</i> , 2020, 265, 106439.	1.5	9
83	Recent Advances on Graphene-Based Gas Sensors. <i>Russian Journal of Physical Chemistry A</i> , 2020, 94, 2115-2120.	0.1	9
84	Pharmacophore-enabled virtual screening, molecular docking and molecular dynamics studies for identification of potent and selective histone deacetylase 8 inhibitors. <i>Computers in Biology and Medicine</i> , 2020, 123, 103850.	3.9	9
85	Theoretical Studies on Hydroxamic Acids. , 2013, , 19-53.		9
86	Metal ion complexes of thioformin: A density functional study. <i>Polyhedron</i> , 2007, 26, 5301-5308.	1.0	8
87	DFT studies on the acid-catalyzed Curtius reaction: the Schmidt reaction. <i>Structural Chemistry</i> , 2017, 28, 1743-1756.	1.0	8
88	Adsorption of Bromonitromethane over Graphene-Based Substrates: A Density Functional Theory Analysis. <i>ChemistrySelect</i> , 2019, 4, 4967-4974.	0.7	8
89	Combined pharmacophore-guided 3D-QSAR, molecular docking, and virtual screening on bis-benzimidazoles and ter-benzimidazoles as DNA topoisomerase I poisons. <i>Structural Chemistry</i> , 2019, 30, 1185-1201.	1.0	8
90	Theoretical study of the structural features and antioxidant potential of 4-thiazolidinones. <i>Structural Chemistry</i> , 2020, 31, 1599-1608.	1.0	8

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91	Identification of potent human carbonic anhydrase IX inhibitors: a combination of pharmacophore modeling, 3D-QSAR, virtual screening and molecular dynamics simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 4516-4531.	2.0	8
92	A combination strategy of structure-based virtual screening, MM-GBSA, cross docking, molecular dynamics and metadynamics simulations used to investigate natural compounds as potent and specific inhibitors of tumor linked human carbonic anhydrase IX. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 5465-5480.	2.0	8
93	An insight into pyruvate dehydrogenase kinase (PDHK) inhibition through pharmacophore modeling and QSAR studies. <i>Journal of Computational Science</i> , 2014, 5, 558-567.	1.5	7
94	Adsorptive Degradation of Phosmet Using Hierarchically Porous Calcium Oxide : An Experimental and Theoretical Study. <i>ChemistrySelect</i> , 2020, 5, 1235-1246.	0.7	7
95	A theoretical assessment of the structural and electronic features of some retrochalcones. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26797.	1.0	7
96	Theoretical study of unimolecular rearrangements of vinylidenes to acetylenes. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 189-199.	1.0	6
97	Assessment of theoretical methods for the study of hydrogen abstraction kinetics of global warming gas species during their degradation and byproduct formation (IUPAC Technical Report). <i>Pure and Applied Chemistry</i> , 2013, 85, 1901-1918.	0.9	6
98	Theoretical study of the mechanism of the Wolff rearrangement of some diazocarbonyl compounds. <i>Computational and Theoretical Chemistry</i> , 2016, 1094, 32-41.	1.1	6
99	Nanocrystalline Hierarchical ZSM-5: An Efficient Catalyst for the Alkylation of Phenol with Cyclohexene. <i>Journal of Nanoscience and Nanotechnology</i> , 2018, 18, 5404-5413.	0.9	6
100	Theoretical study of the mechanism of proton transfer in tautomeric systems: Alloxan. <i>Journal of Chemical Sciences</i> , 2001, 113, 297-306.	0.7	5
101	Theoretical studies on the mechanism of radioprotection by Hoechst 33258 derivatives. <i>Computational and Theoretical Chemistry</i> , 2004, 668, 243-248.	1.5	5
102	Metal Ion Selectivity of Kojate Complexes: A Theoretical Study. <i>Journal of Theoretical Chemistry</i> , 2013, 1-9.	1.5	5
103	DFT study of carbaryl pesticide adsorption on vacancy and nitrogen-doped graphene decorated with platinum clusters. <i>Structural Chemistry</i> , 2021, 32, 1541-1551.	1.0	5
104	Synthetic methods and biological applications of retrochalcones isolated from the root of <i>Glycyrrhiza</i> species: A review. <i>Results in Chemistry</i> , 2021, 3, 100216.	0.9	5
105	QSAR studies on the mechanism of radioprotection by Hoechst 33258 analogues. <i>Computational and Theoretical Chemistry</i> , 2005, 714, 35-42.	1.5	4
106	Theoretical study of the thermal unimolecular rearrangement of fluoroethylidenes. <i>International Journal of Quantum Chemistry</i> , 1992, 44, 363-377.	1.0	3
107	Preparation, properties and infrared spectral studies of N-(p-ethylphenyl)thiobenzohydroxamic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 68, 1362-1369.	2.0	3
108	Negative ion Wolff rearrangement of some diazoketones: A theoretical mechanistic study. <i>Computational and Theoretical Chemistry</i> , 2017, 1106, 50-57.	1.1	3

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109	Theoretical investigation of the structural and electronic features of SLC-0111, a novel inhibitor of human carbonic anhydrase IX, and its anion. <i>Structural Chemistry</i> , 2021, 32, 1843-1856.	1.0	3
110	Theoretical study of the excited singlet and triplet states of alloxan. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 502-509.	1.0	2
111	Effects of increasing number of rings on the ion sensing ability of CdSe quantum dots: a theoretical study. <i>Journal of Nanoparticle Research</i> , 2018, 20, 1.	0.8	2
112	DFT studies on storage and adsorption capacities of gases on MOFs. <i>Physical Sciences Reviews</i> , 2018, 3, .	0.8	2
113	Theoretical investigation of organotin(IV) complexes of substituted benzohydroxamic acids. <i>Computational and Theoretical Chemistry</i> , 2018, 1138, 57-65.	1.1	2
114	Combined approach of homology modeling, molecular dynamics, and docking: computer-aided drug discovery. <i>Physical Sciences Reviews</i> , 2019, 4, .	0.8	2
115	A DFT-D2 study on Mo <sub>4</sub> -xCo <sub>x</sub> (x = 0-3) cluster-decorated graphene and the adsorption of SO <sub>2</sub> F <sub>2</sub> and SOF <sub>2</sub> on Mo <sub>4</sub> -decorated graphene. <i>Journal of Nanoparticle Research</i> , 2020, 22, 1.	0.8	2
116	Computational Studies on Reactions of Some Organic Azides with C-H Bonds. <i>ChemistrySelect</i> , 2021, 6, 4368-4381.	0.7	2
117	A comparative study of different docking methodologies to assess the protein-ligand interaction for the <i>E. coli</i> MurB enzyme. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 11229-11238.	2.0	2
118	C <sub>3</sub> H <sub>4</sub> : Theoretical study of structures and stabilities of isomers. , 1996, 58, 389.		2
119	Size-dependent structural and electronic properties of stoichiometric II-VI quantum dots and gas sensing ability of CdSe quantum dots: a DFT study. <i>Journal of Nanoparticle Research</i> , 2022, 24, .	0.8	2
120	The selective removal of Congo red using dumbbell-shaped hierarchically porous Ca-Mg mixed oxide. <i>Applied Surface Science Advances</i> , 2022, 8, 100221.	2.9	2
121	Density functional (DFT) study of acyloxy carbene-carbene rearrangements. <i>Computational and Theoretical Chemistry</i> , 2003, 626, 187-194.	1.5	1
122	Spectral and theoretical studies of N-p-(ethylbenzene)thiobenzohydroxamic acid metal chelates. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 62, 819-825.	2.0	1
123	A novel non-TOPO route for the synthesis of colloidal CdSe quantum dots with high luminescence and stability. , 2007, , .		1
124	DFT STUDY OF SOME TRIVALENT d- AND f-BLOCK METAL ION COMPLEXES OF ALLOXAN. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1350052.	1.8	1
125	Rearrangements in radical cations of diazoketones: A DFT mechanistic study. <i>Computational and Theoretical Chemistry</i> , 2018, 1134, 30-36.	1.1	1
126	Pharmacophore modeling, 3D-QSAR and molecular docking studies of quinazolines and aminopyridines as selective inhibitors of inducible nitric oxide synthase. <i>Journal of Theoretical and Computational Chemistry</i> , 2019, 18, 1950002.	1.8	1



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127	Chem-bioinformatic approach for drug discovery. , 2021, , 207-243.		1
128	Decontamination of chloropicrin (PS) and its analogues using graphene and modified graphene surfaces: a computational study. Structural Chemistry, 2021, 32, 1883-1892.	1.0	1
129	<i>In silico</i> study of the synergistic anti-tumor effect of hybrid topoisomerase-HDAC inhibitors. Pure and Applied Chemistry, 2021, 93, 1213-1228.	0.9	1
130	Unimolecular rearrangements of ethylnitrene: An exploratory theoretical study. Journal of Computational Chemistry, 1991, 12, 1211-1216.	1.5	0
131	Tertiary Butylation of Aniline Over Nanosized Zeolite Beta Catalyst. Journal of Nanoscience and Nanotechnology, 2018, 18, 7960-7968.	0.9	0
132	6. DFT studies on storage and adsorption capacities of gases on MOFs. , 2018, , 83-112.		0