Ehsan Zahedi

List of Publications by Year
in descending order

90	799	623734	642732
papers	citations	14 h-index	23 g-index

90	90	90	966
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The cross-substitution effect of tantalum on the visible-light-driven water oxidation activity of BaNbO₂N crystals grown directly by an NH₃-assisted flux method. Journal of Materials Chemistry A, 2016, 4, 12807-12817.	10.3	50
2	New Dionâ€“Jacobson Phase Three-Layer Perovskite CsBa₂Ta₃O₁₀ and Its Conversion to Nitrided Ba₂Ta₃O₁₀ Nanosheets via a Nitridationâ€“Protonationâ€“Intercalationâ€“Exfoliation Route for Water Splitting. Crystal Growth and Design, 2016, 16, 2302-2308.	3.0	47
3	Following the Molecular Mechanism of Decarbonylation of Unsaturated Cyclic Ketones Using Bonding Evolution Theory Coupled with NCI Analysis. Journal of Physical Chemistry A, 2017, 121, 8504-8517.	2.5	40
4	Hydrostatic pressure effects on the electronic, optical, and photocatalytic properties of ribbon-like Bi2S3: A DFT study. Superlattices and Microstructures, 2015, 81, 49-63.	3.1	32
5	Two-step synthesis and visible-light-driven photocatalytic water oxidation activity of AW(O,N)3 (A= Sr,) Tj ETQq1 1 0.784314 rgBT /Ov	6.2	31
6	Atmospheric oxidation reactions of imidazole initiated by hydroxyl radicals: kinetics and mechanism of reactions and atmospheric implications. Physical Chemistry Chemical Physics, 2019, 21, 8445-8456.	2.8	31
7	DFT study of structural, elastic properties and thermodynamic parameters of Bi2S3 under hydrostatic pressures. Computational Materials Science, 2015, 101, 301-312.	3.0	28
8	Adsorption of NH3 and NO2 molecules on C48B6N6 heterofullerene: A DFT study on electronic properties. Physica B: Condensed Matter, 2011, 406, 3704-3709.	2.7	26
9	Tuning the morphological structure, light absorption, and photocatalytic activity of Bi2WO6 and Bi2WO6-BiOCl through cerium doping. Arabian Journal of Chemistry, 2020, 13, 2844-2857.	4.9	26
10	The contrasting effect of the Ta/Nb ratio in (111)-layered B-site deficient hexagonal perovskite Ba₅Nb_{4â^'x}Ta_xO₁₅ crystals on visible-light-induced photocatalytic water oxidation activity of their oxynitride derivatives. Dalton Transactions, 2016, 45, 12559-12568.	3.3	24
11	First-Principles Investigations of the Structure, Electronic, and Optical Properties of Mullite-Type Orthorhombic Bi₂M₄O₉ (M = Al³⁺, Ga³⁺). Inorganic Chemistry, 2016, 55, 4824-4835.	4.0	23
12	Effect of tube radius on the exohedral chemical functionalization of boron-nitride zigzag nanotubes with NH3. Physica B: Condensed Matter, 2012, 407, 3841-3848.	2.7	20
13	A density functional study of NBO, NICS and 14N NQR parameters of 5-methylcytosine tautomers in the gas phase. Computational and Theoretical Chemistry, 2009, 905, 101-105.	1.5	19
14	Kinetic and mechanistic insight into the OH â€“initiated atmospheric oxidation of 2,3,7,8-tetrachlorodibenzo-p-dioxin via OH â€“addition and hydrogen abstraction pathways: A theoretical investigation. Science of the Total Environment, 2019, 679, 106-114.	8.0	17
15	Electronic, optical and photocatalytic properties of three-layer perovskite Dionâ€“Jacobson phase CsBa₂M₃O₁₀(M = Ta, Nb): a DFT study. RSC Advances, 2015, 5, 88725-88735.	3.6	15
16	Molecular Dynamics Simulation of Wetting and Interfacial Properties of Multicationic Ionic Liquid Nanodroplets on Boron Nitride Monolayers: A Comparative Approach. Journal of Physical Chemistry C, 2019, 123, 13551-13560.	3.1	15
17	Understanding the kinetics and molecular mechanism of the Curtius rearrangement of 3-oxocyclobutane-1-carbonyl azide. Computational and Theoretical Chemistry, 2018, 1130, 121-129.	2.5	14
18	Structural and Electronic Properties of Ammonia Adsorption on the C₃₀B₁₅N₁₅ Heterofullerene: A Density Functional Theory Study. Journal of Computational and Theoretical Nanoscience, 2011, 8, 2159-2165.	0.4	13

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19	Theoretical study on the mechanisms and kinetics of the Î²-elimination of 2,2-dihaloethyltrihalosilanes (XÂ=ÂF, Cl, Br) compounds: a DFT study along with a natural bond orbital analysis. Reaction Kinetics, Mechanisms and Catalysis, 2018, 124, 27-44.	1.7	13
20	Adsorption of nitrogen dioxide on C30B15N15 heterofullerene: AIM and NBO study via DFT. Comptes Rendus Chimie, 2013, 16, 189-194.	0.5	11
21	A DFT Study of NBO and NICS Analysis of the Allylic Rearrangements (the Claisen and Thio-Claisen) Tj ETQq1 1 0.784314 rgBT /Overlock the Related Elements, 2010, 186, 159-170.	1.6	10
22	A DFT study of carbon nanobuds. European Physical Journal B, 2011, 82, 147-152.	1.5	10
23	Mechanism and regioselectivity of 1,3-dipolar cycloaddition reactions of sulphur-centred dipoles with furan-2,3-dione: A theoretical study using DFT. Journal of Chemical Sciences, 2014, 126, 293-302.	1.5	10
24	Density functional theory study of electric field effects on the isomerization of a photochromic molecular switch based on 1,2-dithienylethene. Canadian Journal of Chemistry, 2014, 92, 317-323.	1.1	10
25	Understanding the molecular mechanism of thio-Claisen rearrangement of allyl phenyl sulfide and allyl vinyl sulfide using bonding evolution theory coupled with NCI analysis. Journal of Sulfur Chemistry, 2018, 39, 350-366.	2.0	10
26	The influence of NH3 -attaching on the NMR parameters in the zigzag BN nanotube. Superlattices and Microstructures, 2011, 49, 169-175.	3.1	8
27	Understanding the kinetics of thermal decomposition of 2,3-epoxy-2,3-dimethylbutane using RRKM theory. RSC Advances, 2016, 6, 91882-91892.	3.6	8
28	Understanding the kinetics and mechanism of thermal cheletropic elimination of N2 from (2,5-dihydro-1H-pyrrol-1-ium-1-ylidene) amide using RRKM and ELF theories. Research on Chemical Intermediates, 2017, 43, 1575-1590.	2.7	8
29	Regioselectivity of 1,3-dipolar cycloadditions between aryl azides and an electron-deficient alkyne through DFT reactivity descriptors. Research on Chemical Intermediates, 2017, 43, 767-782.	2.7	8
30	Unravelling the kinetics and molecular mechanism of the degenerate Cope rearrangement of bullvalene. New Journal of Chemistry, 2020, 44, 6543-6552.	2.8	8
31	A molecular electron density theory (MEDT) study of the role of halogens (X₂=) Tj ETQq1 1 0.784314 rgBT /Overlock 10 reactions. New Journal of Chemistry, 2020, 44, 19002-19012.	2.8	8
32	Effect of tube radius on the electronic and magnetic properties of finite boron nitride zigzag nanotubes using DFT. Physica E: Low-Dimensional Systems and Nanostructures, 2011, 44, 179-185.	2.7	7
33	Molecular Dynamics Simulation of Boron Nitride Nanotube as a Drug Carrier. Arabian Journal for Science and Engineering, 2014, 39, 6737-6742.	1.1	7
34	DFT STUDY OF CO AND NO ADSORPTION ON BORON NITRIDE (BN)_{n = 3 - 5} NANOCLUSTERS. Surface Review and Letters, 2015, 22, 1550005.	1.1	7
35	Effective masses, electronic and optical properties of (111)-layered B-site deficient hexagonal perovskite Ba5M4O15 (M = Ta, Nb): a DFT study using HSE06. RSC Advances, 2016, 6, 61150-61161.	3.6	7
36	Kinetic and mechanistic study on the pyrolysis of 1,3-dihydroisothianaphthene-2,2-dioxide toward benzocyclobutene using RRKM and BET theories. Chemical Physics, 2017, 483-484, 12-25.	1.9	7

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37	Understanding the kinetics and molecular mechanism of unimolecular gas phase thermal decomposition of the Î±-ketoester methyl benzoylformate using RRKM and BET theories. Journal of Molecular Graphics and Modelling, 2019, 87, 22-29.	2.4	7
38	Solvent effects on stability and 15N NMR shielding of 5-methylcytosine tautomers: A theoretical approach. Computational and Theoretical Chemistry, 2009, 899, 94-97.	1.5	6
39	The comparative study in transport properties of furan, thiophene and selenophene dithiols in nano electronic. Superlattices and Microstructures, 2011, 50, 386-399.	3.1	6
40	Size-dependent electronic structures of boron carbonitride (BC2N) nanotubes. A DFT approach. Superlattices and Microstructures, 2011, 50, 491-500.	3.1	6
41	A DFT studies of structural and quadrupole coupling constants properties in C-doped BeO nanotubes. Superlattices and Microstructures, 2011, 50, 539-548.	3.1	6
42	DFT-NEGF study of transport properties and NDR behavior in fused furan and thiophene dimmers. Physica B: Condensed Matter, 2012, 407, 4503-4511.	2.7	6
43	The unimolecular thermal decomposition of oxetane and its methyl derivatives: An Ab initio and RRKM calculations. Russian Journal of Physical Chemistry A, 2012, 86, 1245-1249.	0.6	6
44	Currentâ€“voltage characteristics through dithienylcyclopentene: A NEGF-DFT study. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 61, 1-8.	2.7	6
45	Adsorption of carbon monoxide on boroxol-ring-doped zigzag boron nitride nanotube: Electronic study via DFT. European Physical Journal Plus, 2016, 131, 1.	2.6	6
46	A firstâ€“principles study on polar hexagonal Cs 2 Te M 3 O 12 (M = W, Mo): New visibleâ€“light responsive photocatalyst. Journal of Solid State Chemistry, 2017, 252, 129-137.	2.9	6
47	Kinetic and mechanistic insight into the formation of amphetamine using the Leuckartâ€“Wallach reaction and interaction of the drug with GpCÂ·CpG base-pair step of DNA: a DFT study. Monatshefte FÃ¼r Chemie, 2018, 149, 1045-1057.	1.8	6
48	Reaction mechanisms and kinetics of the Î²-elimination processes of compounds CHF2CH2SiF Me3â€“(nâ€‰=â€‰0â€“3): DFT and CBS-QB3 methods using Rice-Ramsperger-Kassel-Marcus and transition state theories. Journal of Fluorine Chemistry, 2018, 216, 71-80.	1.7	6
49	NBO and NICS analysis of the allylic rearrangements (the Cope and 3-aza-Cope rearrangements) of hexa-1,5-diene and N-vinylprop-2-en-1-amine: A DFT study. Open Chemistry, 2010, 8, 1097-1104.	1.9	5
50	Kinetic and thermodynamic study of the substituent effect on the amino-Claisen rearrangement ofpara-substitutedN-allyl-N-arylamine: a Hammett study via DFT. Molecular Simulation, 2010, 36, 978-985.	2.0	5
51	Ammonia adsorption on the C30B15N15 heterofullerene: DFT study of nuclear magnetic shielding and electric field gradient tensors of N and B nuclei. Physica B: Condensed Matter, 2011, 406, 1592-1597.	2.7	5
52	Theoretical Study and Nbo Analysis of the Kinetics and Mechanism of the Gas Phase Elimination Reactions of 2-Chloroethylsilane and Derivatives. Progress in Reaction Kinetics and Mechanism, 2012, 37, 76-89.	2.1	5
53	DFT STUDY OF HYDROGEN STORAGE ON Li- AND Na-DOPED C59B HETEROFULLERENE. Surface Review and Letters, 2014, 21, 1450047.	1.1	5
54	Quasi-RRHO approximation and DFT study for understanding the mechanism and kinetics of nitration reaction of benzonitrile with nitronium ion. Computational and Theoretical Chemistry, 2021, 1199, 113209.	2.5	5

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55	A computational investigation of carbon-doped beryllium monoxide nanotubes. Open Chemistry, 2012, 10, 96-104.	1.9	4
56	Theoretical study on the elimination kinetics in the gas phase of allyl methyl compounds. Monatshefte FÃ¼r Chemie, 2018, 149, 1389-1400.	1.8	4
57	Aziridination of Aromatic Aldimines Through Stabilized Ammonium Ylides: A Molecular Electron Density Theory Study. European Journal of Organic Chemistry, 2019, 2019, 1605-1613.	2.4	4
58	[3 + 2] cycloaddition reaction ofN,Nâ€²cyclic azomethine imines toward highly electronâ€deficient nitroalkenes: A molecular electron density theory study. Journal of Physical Organic Chemistry, 2019, 32, e3925.	1.9	4
59	Zinc Oxide/Graphene Oxide as a Robust Active Catalyst for Direct Oxidative Synthesis of Nitriles from Alcohols in Water. Catalysis Letters, 2022, 152, 1895-1903.	2.6	4
60	Ab Initio Study and Nbo Analysis of the Unimolecular Decomposition Kinetics of 2,2-Dimethyloxetane. Progress in Reaction Kinetics and Mechanism, 2012, 37, 277-290.	2.1	3
61	DFT Study of NBO, NICS and ¹⁴N NQR Parameters of Guanine Tautomers in the Gas Phase. Zeitschrift Fur Physikalische Chemie, 2012, 226, 47-57.	2.8	3
62	DFT Calculations of the Elimination Kinetics of Silacyclobutanes and its Methyl Derivatives in the Gas-Phase. Phosphorus, Sulfur and Silicon and the Related Elements, 2012, 187, 619-631.	1.6	3
63	Mechanism and Regioselectivity of the 1,3-Dipolar Cycloaddition of Methyleneamine N-Oxide with Cyclopent-3-Ene-1,2-Dione and its Aza, Oxa and Thia Analogues: A Dft Approach. Progress in Reaction Kinetics and Mechanism, 2012, 37, 90-102.	2.1	3
64	Mechanism and regioselectivity of the 1,3â€dipolar cycloaddition of thiocarbonyl Sâ€imide with cyclopentâ€3â€eneâ€1,2â€dione and methoxyethene: a density functional theory approach. Journal of Physical Organic Chemistry, 2012, 25, 748-753.	1.9	3
65	Isomerisation Reactions of Î±-Methyl Allyl [Acetate, Trifluoroacetate]: Theoretical Study. Progress in Reaction Kinetics and Mechanism, 2013, 38, 249-265.	2.1	3
66	Reaction mechanisms and kinetics of the elimination processes of 2-chloroethylsilane and derivatives: A DFT study using CTST, RRKM, and BET theories. Chemical Physics, 2017, 485-486, 140-148.	1.9	3
67	Exohedral chemical functionalization of C48B6N6 with NH3: Binding energies and electronic structures of C48B6N6â€“(NH3)n=1â^'6. Superlattices and Microstructures, 2012, 51, 290-299.	3.1	2
68	Transport properties of a single-molecular diode with one backbone, and two backbones in parallel: Frontier orbital analysis and NEGF-DFT study. European Physical Journal Plus, 2015, 130, 1.	2.6	2
69	Dielsâ€“Alder Reactions of Î±-Cyano Î±,Î²-Unsaturated Ketones with 2-Methyl-1,3-Butadiene: DFT Study of Mechanism, Reactivity and Regioselectivity. Progress in Reaction Kinetics and Mechanism, 2015, 40, 177-189.	2.1	2
70	Unraveling the kinetics and molecular mechanism of gas phase pyrolysis of cubane to [8]annulene. RSC Advances, 2020, 10, 32730-32739.	3.6	2
71	Atmospheric Oxidation Reactions of Methyl Salicylate as Green Leaf Volatiles by OH Radical: Theoretical Kinetics and Mechanism. ChemistrySelect, 2020, 5, 12535-12547.	1.5	2
72	Insights into the kinetics and molecular mechanism of the Newmanâ€“Kwart rearrangement. New Journal of Chemistry, 2021, 45, 16978-16988.	2.8	2

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73	Control aromaticity in the thermal decomposition of 2,5-dihydrofuran, 2,5-dihydrothiophene and 3-pyrroline: a kinetic and thermodynamic study via DFT. Reaction Kinetics, Mechanisms and Catalysis, 2011, 102, 21-35.	1.7	1
74	Kinetic Study and NBO Analysis of the Dehydrogenation Mechanism of Five-membered Ring Heterocyclic 2,5-Dihydro-[furan, thiophene, selenophene. Chinese Journal of Chemistry, 2011, 29, 2249-2256.	4.9	1
75	Dft Study of Allylic Rearrangements (Cope Rearrangements) of Substituted Hexa-L,5-Dienes: Nbo and Nics Analysis. Progress in Reaction Kinetics and Mechanism, 2011, 36, 166-177.	2.1	1
76	A Theoretical Study of NBO, NICS, and ¹⁴N NQR Parameters of Adenine Tautomers in the Gas Phase via DFT. Journal of Heterocyclic Chemistry, 2012, 49, 782-788.	2.6	1
77	Mechanism and regioselectivity of the reversible Dielsâ€“Alder cycloaddition of 2-methyl-1,3 butadiene with C 48 B 6 N 6 heterofullerene: A DFT approach. Journal of Molecular Graphics and Modelling, 2014, 53, 212-220.	2.4	1
78	Comparative Investigation of the Stabilities of Indene and Isoindene and the Their Heteroanalogs (N,O,S) Using Computational Methods. Phosphorus, Sulfur and Silicon and the Related Elements, 2014, 189, 1367-1377.	1.6	1
79	Theoretical study of the pressure dependent rate constants of the thermal decomposition of Î²-propiolactone. Arabian Journal of Chemistry, 2015, 8, 644-647.	4.9	1
80	Adsorption properties of boroxol ring doped zigzag boron nitride nanotube toward NO molecule using DFT. International Journal of Modern Physics B, 2016, 30, 1650101.	2.0	1
81	First-principles investigation of the equation of state and elastic properties of perovskite-type SrW(O,N)3 under hydrostatic pressures up to 139 GPa. European Physical Journal B, 2017, 90, 1.	1.5	1
82	A Theoretical Study on the Degenerate Cope Rearrangement of Hypostrophene Using the RRKM Theory and Topological Approaches. ChemistrySelect, 2021, 6, 1607-1615.	1.5	1
83	DFT Insight into the Kinetics and Mechanism of the OH . â€Ինitiated Atmospheric Oxidation of Catechol: OH . Addition and Hydrogen Abstraction Pathways. ChemistrySelect, 2021, 6, 3875-3883.	1.5	1
84	Closer Investigation of the Kinetics and Mechanism of Spirovinylcyclopropyl Oxindole Reaction with 3Î£â€“g-O2 by Topological Approaches and Unraveling the Role of the I2 Catalyst. Journal of Physical Chemistry A, 2021, 125, 6913-6926.	2.5	1
85	A comprehensive theoretical analysis of Curtius rearrangement of syn-syn and syn-anti conformers of oxalyl diazide. Journal of Molecular Graphics and Modelling, 2021, 109, 108012.	2.4	1
86	Kinetics and molecular mechanism of the Schonberg rearrangement. Computational and Theoretical Chemistry, 2022, 1208, 113585.	2.5	1
87	Theoretical investigation on the mechanism and kinetics of the OHâ€¢â€'initiated atmospheric degradation of p-chloroaniline via OHâ€¢â€'addition and hydrogen abstraction pathways. Journal of Molecular Graphics and Modelling, 2022, 114, 108198.	2.4	1
88	Theoretical study of proton transfer in ammoniaâ€“hydrogen halides in the presence of methanol. Research on Chemical Intermediates, 2013, 39, 3303-3317.	2.7	0
89	Influence of NO2 attachment on the nuclear magnetic shielding tensors of N and B nuclei in C30B15N15 heterofullerene: a DFT study. Research on Chemical Intermediates, 2013, 39, 3843-3857.	2.7	0
90	The Allylic Rearrangements (Claisen and Thio-Claisen) and Decomposition Reactions of Allyl Formate and its Sulfur Analogue: Density Function Theory Study and Nucleus-Independent Chemical Shifts. Progress in Reaction Kinetics and Mechanism, 2013, 38, 171-182.	2.1	0