

Ehsan Zahedi

List of Publications by Year in descending order

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90
papers

799
citations

623734

14
h-index

642732

23
g-index

90
all docs

90
docs citations

90
times ranked

966
citing authors

#	ARTICLE	IF	CITATIONS
1	Zinc Oxide/Graphene Oxide as a Robust Active Catalyst for Direct Oxidative Synthesis of Nitriles from Alcohols in Water. <i>Catalysis Letters</i> , 2022, 152, 1895-1903.	2.6	4
2	Kinetics and molecular mechanism of the Schonberg rearrangement. <i>Computational and Theoretical Chemistry</i> , 2022, 1208, 113585.	2.5	1
3	Theoretical investigation on the mechanism and kinetics of the OH-initiated atmospheric degradation of p-chloroaniline via OH-addition and hydrogen abstraction pathways. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 114, 108198.	2.4	1
4	Insights into the kinetics and molecular mechanism of the Newman-Kwart rearrangement. <i>New Journal of Chemistry</i> , 2021, 45, 16978-16988.	2.8	2
5	A Theoretical Study on the Degenerate Cope Rearrangement of Hypostrophene Using the RRKM Theory and Topological Approaches. <i>ChemistrySelect</i> , 2021, 6, 1607-1615.	1.5	1
6	DFT Insight into the Kinetics and Mechanism of the OH-initiated Atmospheric Oxidation of Catechol: OH Addition and Hydrogen Abstraction Pathways. <i>ChemistrySelect</i> , 2021, 6, 3875-3883.	1.5	1
7	Quasi-RRHO approximation and DFT study for understanding the mechanism and kinetics of nitration reaction of benzonitrile with nitronium ion. <i>Computational and Theoretical Chemistry</i> , 2021, 1199, 113209.	2.5	5
8	Closer Investigation of the Kinetics and Mechanism of Spirovinylcyclopropyl Oxindole Reaction with $3\text{I}_2\text{-g-O}_2$ by Topological Approaches and Unraveling the Role of the I2 Catalyst. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6913-6926.	2.5	1
9	A comprehensive theoretical analysis of Curtius rearrangement of syn-syn and syn-anti conformers of oxalyl diazide. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 109, 108012.	2.4	1
10	Tuning the morphological structure, light absorption, and photocatalytic activity of Bi ₂ WO ₆ and Bi ₂ WO ₆ -BiOCl through cerium doping. <i>Arabian Journal of Chemistry</i> , 2020, 13, 2844-2857.	4.9	26
11	Unraveling the kinetics and molecular mechanism of gas phase pyrolysis of cubane to [8]annulene. <i>RSC Advances</i> , 2020, 10, 32730-32739.	3.6	2
12	Atmospheric Oxidation Reactions of Methyl Salicylate as Green Leaf Volatiles by OH Radical: Theoretical Kinetics and Mechanism. <i>ChemistrySelect</i> , 2020, 5, 12535-12547.	1.5	2
13	Unravelling the kinetics and molecular mechanism of the degenerate Cope rearrangement of bullvalene. <i>New Journal of Chemistry</i> , 2020, 44, 6543-6552.	2.8	8
14	A molecular electron density theory (MEDT) study of the role of halogens (X_{2}) reactions. <i>New Journal of Chemistry</i> , 2020, 44, 19002-19012.	2.8	8
15	Molecular Dynamics Simulation of Wetting and Interfacial Properties of Multicationic Ionic Liquid Nanodroplets on Boron Nitride Monolayers: A Comparative Approach. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13551-13560.	3.1	15
16	Kinetic and mechanistic insight into the OH-initiated atmospheric oxidation of 2,3,7,8-tetrachlorodibenzo-p-dioxin via OH-addition and hydrogen abstraction pathways: A theoretical investigation. <i>Science of the Total Environment</i> , 2019, 679, 106-114.	8.0	17
17	Atmospheric oxidation reactions of imidazole initiated by hydroxyl radicals: kinetics and mechanism of reactions and atmospheric implications. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8445-8456.	2.8	31
18	Aziridination of Aromatic Aldimines Through Stabilized Ammonium Ylides: A Molecular Electron Density Theory Study. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 1605-1613.	2.4	4

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19	[3 + 2] cycloaddition reaction of N,N-dicyclic azomethine imines toward highly electron-deficient nitroalkenes: A molecular electron density theory study. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3925.	1.9	4
20	Understanding the kinetics and molecular mechanism of unimolecular gas phase thermal decomposition of the β -ketoester methyl benzoylformate using RRKM and BET theories. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 87, 22-29.	2.4	7
21	Kinetic and mechanistic insight into the formation of amphetamine using the Leuckart-Wallach reaction and interaction of the drug with GpCpG base-pair step of DNA: a DFT study. <i>Monatshefte für Chemie</i> , 2018, 149, 1045-1057.	1.8	6
22	Understanding the molecular mechanism of thio-Claisen rearrangement of allyl phenyl sulfide and allyl vinyl sulfide using bonding evolution theory coupled with NCI analysis. <i>Journal of Sulfur Chemistry</i> , 2018, 39, 350-366.	2.0	10
23	Theoretical study on the mechanisms and kinetics of the β -elimination of 2,2-dihaloethyltrihalosilanes (X= F, Cl, Br) compounds: a DFT study along with a natural bond orbital analysis. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2018, 124, 27-44.	1.7	13
24	Understanding the kinetics and molecular mechanism of the Curtius rearrangement of 3-oxocyclobutane-1-carbonyl azide. <i>Computational and Theoretical Chemistry</i> , 2018, 1130, 121-129.	2.5	14
25	Reaction mechanisms and kinetics of the β -elimination processes of compounds CHF ₂ CH ₂ SiF ₂ Me ₃ (n=0,1,2,3): DFT and CBS-QB3 methods using Rice-Ramsperger-Kassel-Marcus and transition state theories. <i>Journal of Fluorine Chemistry</i> , 2018, 216, 71-80.	1.7	6
26	Theoretical study on the elimination kinetics in the gas phase of allyl methyl compounds. <i>Monatshefte für Chemie</i> , 2018, 149, 1389-1400.	1.8	4
27	Reaction mechanisms and kinetics of the elimination processes of 2-chloroethylsilane and derivatives: A DFT study using CTST, RRKM, and BET theories. <i>Chemical Physics</i> , 2017, 485-486, 140-148.	1.9	3
28	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. <i>European Physical Journal B</i> , 2017, 90, 1.	1.5	1
29	A first-principles study on polar hexagonal Cs ₂ TeM ₃ O ₁₂ (M = W, Mo): New visible-light responsive photocatalyst. <i>Journal of Solid State Chemistry</i> , 2017, 252, 129-137.	2.9	6
30	Following the Molecular Mechanism of Decarbonylation of Unsaturated Cyclic Ketones Using Bonding Evolution Theory Coupled with NCI Analysis. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8504-8517.	2.5	40
31	Kinetic and mechanistic study on the pyrolysis of 1,3-dihydroisothianaphthene-2,2-dioxide toward benzocyclobutene using RRKM and BET theories. <i>Chemical Physics</i> , 2017, 483-484, 12-25.	1.9	7
32	Understanding the kinetics and mechanism of thermal cheletropic elimination of N ₂ from (2,5-dihydro-1H-pyrrol-1-ium-1-ylidene) amide using RRKM and ELF theories. <i>Research on Chemical Intermediates</i> , 2017, 43, 1575-1590.	2.7	8
33	Regioselectivity of 1,3-dipolar cycloadditions between aryl azides and an electron-deficient alkyne through DFT reactivity descriptors. <i>Research on Chemical Intermediates</i> , 2017, 43, 767-782.	2.7	8
34	The cross-substitution effect of tantalum on the visible-light-driven water oxidation activity of BaNbO ₂ N crystals grown directly by an NH ₃ -assisted flux method. <i>Journal of Materials Chemistry A</i> , 2016, 4, 12807-12817.	10.3	50
35	First-Principles Investigations of the Structure, Electronic, and Optical Properties of Mullite-Type Orthorhombic Bi ₂ M ₄ O ₉ (M = Al ³⁺ , Ga ³⁺). <i>Inorganic Chemistry</i> , 2016, 55, 4824-4835.	4.0	23
36	Two-step synthesis and visible-light-driven photocatalytic water oxidation activity of AW(O,N) ₃ (A= Sr, Tj ETQq0 0 0,rgBT /Overlock 10	6.2	31

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37	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
38	The contrasting effect of the Ta/Nb ratio in (111)-layered B-site deficient hexagonal perovskite $Ba_{5-x}Nb_4O_{15}$ crystals on visible-light-induced photocatalytic water oxidation activity of their oxynitride derivatives. Dalton Transactions, 2016, 45, 12559-12568.	3.3	24
39	Effective masses, electronic and optical properties of (111)-layered B-site deficient hexagonal perovskite $Ba_5M_4O_{15}$ (M = Ta, Nb): a DFT study using HSE06. RSC Advances, 2016, 6, 61150-61161.	3.6	7
40	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
41	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
42	New Dionâ€“Jacobson Phase Three-Layer Perovskite $CsBa_2Ta_3O_{10}$ and Its Conversion to Nitrided $Ba_2Ta_3O_{10}$ Nanosheets via a Nitridationâ€“Protonationâ€“Intercalationâ€“Exfoliation Route for Water Splitting. Crystal Growth and Design, 2016, 16, 2302-2308.	3.0	47
43	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
44	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
45	Hydrostatic pressure effects on the electronic, optical, and photocatalytic properties of ribbon-like Bi_2S_3 : A DFT study. Superlattices and Microstructures, 2015, 81, 49-63.	3.1	32
46	DFT study of structural, elastic properties and thermodynamic parameters of Bi_2S_3 under hydrostatic pressures. Computational Materials Science, 2015, 101, 301-312.	3.0	28
47	Dielsâ€“Alder Reactions of $\hat{1},\hat{2}$ -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
48	Electronic, optical and photocatalytic properties of three-layer perovskite Dionâ€“Jacobson phase $CsBa_2M_3O_{10}$ (M = Ta, Nb): a DFT study. RSC Advances, 2015, 5, 88725-88735.	3.6	15
49	Theoretical study of the pressure dependent rate constants of the thermal decomposition of $\hat{1},\hat{2}$ -propiolactone. Arabian Journal of Chemistry, 2015, 8, 644-647.	4.9	1
50	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
51	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
52	Mechanism and regioselectivity of the reversible Dielsâ€“Alder cycloaddition of 2-methyl-1,3 butadiene with $C_{48}B_6N_6$ heterofullerene: A DFT approach. Journal of Molecular Graphics and Modelling, 2014, 53, 212-220.	2.4	1
53	Currentâ€“voltage characteristics through dithienylcyclopentene: A NEGF-DFT study. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 61, 1-8.	2.7	6
54	Molecular Dynamics Simulation of Boron Nitride Nanotube as a Drug Carrier. Arabian Journal for Science and Engineering, 2014, 39, 6737-6742.	1.1	7

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55	DFT STUDY OF HYDROGEN STORAGE ON Li- AND Na-DOPED C59B HETEROFULLERENE. <i>Surface Review and Letters</i> , 2014, 21, 1450047.	1.1	5
56	Comparative Investigation of the Stabilities of Indene and Isoindene and the Their Heteroanalogues (N,O,S) Using Computational Methods. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2014, 189, 1367-1377.	1.6	1
57	Theoretical study of proton transfer in ammonia-hydrogen halides in the presence of methanol. <i>Research on Chemical Intermediates</i> , 2013, 39, 3303-3317.	2.7	0
58	Influence of NO ₂ attachment on the nuclear magnetic shielding tensors of N and B nuclei in C ₃₀ B ₁₅ N ₁₅ heterofullerene: a DFT study. <i>Research on Chemical Intermediates</i> , 2013, 39, 3843-3857.	2.7	0
59	Adsorption of nitrogen dioxide on C ₃₀ B ₁₅ N ₁₅ heterofullerene: AIM and NBO study via DFT. <i>Comptes Rendus Chimie</i> , 2013, 16, 189-194.	0.5	11
60	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. <i>Progress in Reaction Kinetics and Mechanism</i> , 2013, 38, 171-182.	2.1	0
61	Isomerisation Reactions of \pm -Methyl Allyl [Acetate, Trifluoroacetate]: Theoretical Study. <i>Progress in Reaction Kinetics and Mechanism</i> , 2013, 38, 249-265.	2.1	3
62	Ab Initio Study and Nbo Analysis of the Unimolecular Decomposition Kinetics of 2,2-Dimethyloxetane. <i>Progress in Reaction Kinetics and Mechanism</i> , 2012, 37, 277-290.	2.1	3
63	DFT Study of NBO, NICS and ¹⁴ N NQR Parameters of Guanine Tautomers in the Gas Phase. <i>Zeitschrift Fur Physikalische Chemie</i> , 2012, 226, 47-57.	2.8	3
64	DFT Calculations of the Elimination Kinetics of Silacyclobutanes and its Methyl Derivatives in the Gas-Phase. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2012, 187, 619-631.	1.6	3
65	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. <i>Progress in Reaction Kinetics and Mechanism</i> , 2012, 37, 90-102.	2.1	3
66	Theoretical Study and Nbo Analysis of the Kinetics and Mechanism of the Gas Phase Elimination Reactions of 2-Chloroethylsilane and Derivatives. <i>Progress in Reaction Kinetics and Mechanism</i> , 2012, 37, 76-89.	2.1	5
67	DFT-NEGF study of transport properties and NDR behavior in fused furan and thiophene dimmers. <i>Physica B: Condensed Matter</i> , 2012, 407, 4503-4511.	2.7	6
68	Effect of tube radius on the exohedral chemical functionalization of boron-nitride zigzag nanotubes with NH ₃ . <i>Physica B: Condensed Matter</i> , 2012, 407, 3841-3848.	2.7	20
69	A Theoretical Study of NBO, NICS, and ¹⁴ N NQR Parameters of Adenine Tautomers in the Gas Phase via DFT. <i>Journal of Heterocyclic Chemistry</i> , 2012, 49, 782-788.	2.6	1
70	Mechanism and regioselectivity of the 1,3-dipolar cycloaddition of thiocarbonyl imide with cyclopent-3-ene-1,2-dione and methoxyethene: a density functional theory approach. <i>Journal of Physical Organic Chemistry</i> , 2012, 25, 748-753.	1.9	3
71	A computational investigation of carbon-doped beryllium monoxide nanotubes. <i>Open Chemistry</i> , 2012, 10, 96-104.	1.9	4
72	Exohedral chemical functionalization of C ₄₈ B ₆ N ₆ with NH ₃ : Binding energies and electronic structures of C ₄₈ B ₆ N ₆ (NH ₃) _{n=1-6} . <i>Superlattices and Microstructures</i> , 2012, 51, 290-299.	3.1	2

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73	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
74	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
75	Size-dependent electronic structures of boron carbonitride (BC ₂ N) nanotubes. A DFT approach. Superlattices and Microstructures, 2011, 50, 491-500.	3.1	6
76	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
77	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
78	A DFT study of carbon nanobuds. European Physical Journal B, 2011, 82, 147-152.	1.5	10
79	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
80	The influence of NH ₃ -attaching on the NMR parameters in the zigzag BN nanotube. Superlattices and Microstructures, 2011, 49, 169-175.	3.1	8
81	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
82	Ammonia adsorption on the C ₃₀ B ₁₅ N ₁₅ 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
83	Adsorption of NH ₃ and NO ₂ molecules on C ₄₈ B ₆ N ₆ heterofullerene: A DFT study on electronic properties. Physica B: Condensed Matter, 2011, 406, 3704-3709.	2.7	26
84	Dft Study of Allylic Rearrangements (Cope Rearrangements) of Substituted Hexa-1,5-Dienes: Nbo and Nics Analysis. Progress in Reaction Kinetics and Mechanism, 2011, 36, 166-177.	2.1	1
85	Structural and Electronic Properties of Ammonia Adsorption on the C ₃₀ B ₁₅ N ₁₅ Heterofullerene: A Density Functional Theory Study. Journal of Computational and Theoretical Nanoscience, 2011, 8, 2159-2165.	0.4	13
86	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
87	A DFT Study of NBO and NICS Analysis of the Allylic Rearrangements (the Claisen and Thio-Claisen) of the Related Elements, 2010, 186, 159-170.	1.6	10
88	Kinetic and thermodynamic study of the substituent effect on the amino-Claisen rearrangement of <i>para</i> -substituted <i>N</i> -allyl- <i>N</i> -arylamines: a Hammett study via DFT. Molecular Simulation, 2010, 36, 978-985.	2.0	5
89	Solvent effects on stability and ¹⁵ N NMR shielding of 5-methylcytosine tautomers: A theoretical approach. Computational and Theoretical Chemistry, 2009, 899, 94-97.	1.5	6
90	A density functional study of NBO, NICS and ¹⁴ N NQR parameters of 5-methylcytosine tautomers in the gas phase. Computational and Theoretical Chemistry, 2009, 905, 101-105.	1.5	19