Najia Komiha

List of Publications by Year
in descending order

60 papers	834 citations	623734 14 h-index	552781 26 g-index
70 all docs	70 docs citations	70 times ranked	848 citing authors

#	Article	IF	Citations
1	Experimental and theoretical studies for mild steel corrosion inhibition in 1M HCl by two new benzothiazine derivatives. Corrosion Science, 2013, 76, 317-324.	6.6	131
2	One-center expansion for pseudopotential matrix elements. Journal of Computational Chemistry, 1988, 9, 298-302.	3.3	77
3	Dipole moments and orientation polarizabilities of diatomic molecular ions for precision atomic mass measurement. Physical Review A, 2007, 75, .	2.5	48
4	On the stability of cubic phosphorus, P8. Journal of the American Chemical Society, 1985, 107, 7210-7212.	13.7	45
5	A density functional study of alizarin two of its isomers and its transition metals and rare-earth complexes. Computational and Theoretical Chemistry, 2002, 594, 135-145.	1.5	29
6	Removal of oxytetracycline by graphene oxide and Boron-doped reduced graphene oxide: A combined density function Theory, molecular dynamics simulation and experimental study. FlatChem, 2021, 27, 100238.	5.6	28
7	The absorption wavelengths of sulfur chromophors of ultramarines calculated by time-dependent density functional theory. Computational and Theoretical Chemistry, 2006, 801, 63-69.	1.5	25
8	Characterization of Zn^{q+}â€“imidazole (q = 0, 1, 2) organometallic complexes: DFT methods vs. standard and explicitly correlated post-Hartreeâ€“Fock methods. Physical Chemistry Chemical Physics, 2015, 17, 14417-14426.	2.8	23
9	Abâ€…Initio and DFT Studies on CO₂ Interacting with Zn^{q+}â€“Imidazole (q=0, 1, 2) Complexes: Prediction of Charge Transfer through Ïƒâ€•or Ï€â€‘Type Models. ChemPhysChem, 2016, 17, 994-1005.	2.1	22
10	Solvation effects and stabilization of multicharged ions: a case study of ArmBeOq+ complexes. Physical Chemistry Chemical Physics, 2012, 14, 4236.	2.8	20
11	Theoretical study of the 1,3-DC reaction between fluorinated alkynes and azides: Reactivity indices, transition structures, IGM and ELF analysis. Journal of Molecular Graphics and Modelling, 2020, 94, 107458.	2.4	20
12	MEDT study of the 1,3-DC reaction of diazomethane with Psilostachyin and investigation about the interactions of some pyrazoline derivatives with protease (Mpro) of nCoV-2. Journal of Molecular Graphics and Modelling, 2021, 102, 107763.	2.4	20
13	Theoretical Study of the CO₂ Adsorption by Zeolitic Imidazolate Frameworks (ZIFs). Journal of Physical Chemistry C, 2017, 121, 20259-20265.	3.1	19
14	Electronic states of BP, BP+, BPâ^', B2P2, and. Chemical Physics, 2008, 346, 1-7.	1.9	18
15	The photophysical properties and electronic structures of bis[1]benzothieno[6,7-d:6â€²,7â€²-dâ€²]benzo[1,2-b:4,5-bâ€²]dithiophene (BBTBDT) derivatives as hole-transporting materials for organic light-emitting diodes (OLEDs). New Journal of Chemistry, 2019, 43, 15899-15909.	2.8	17
16	Ab initio and DFT studies on the mechanism of the 1,3-dipolar cycloaddition reaction between nitrone and sulfonylethene chloride. Computational and Theoretical Chemistry, 2003, 620, 271-281.	1.5	15
17	Etude DFT du mÃ©canisme des rÃ©actions de cycloaddition dipolaire-1,3 de la C,N-diphÃ©nylnitrone avec des dipolarophiles fluorÃ©s de type Ã©thylÃ©nique et acÃ©tylÃ©nique. Journal of Fluorine Chemistry, 2002, 114, 81-89.	1.7	14
18	DFT study of the mechanism and stereoselectivity of the 1,3-dipolar cycloaddition between pyrroline-1-oxide and methyl crotonate. Journal of Chemical Sciences, 2014, 126, 283-292.	1.5	14

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19	Structural and spectroscopic characterization of methyl isocyanate, methyl cyanate, methyl fulminate, and acetonitrile N-oxide using highly correlated ab initio methods. Journal of Chemical Physics, 2016, 145, 124309.	3.0	14
20	Diabatic research of resonant states in MO-CI calculations of negative ions. Journal of Physics B: Atomic and Molecular Physics, 1987, 20, 4375-4391.	1.6	13
21	Structure, Spectroscopy, and Bonding within the Zn^{q+}â€“Imidazole_n (q = 0, 1, 2; n = 1â€“4) Clusters and Implications for Zeolitic Imidazolate Frameworks and Znâ€“Enzymes. Journal of Physical Chemistry A, 2015, 119, 11928-11940.	2.5	13
22	Computational study of the 1,3-dipolar cycloaddition between methyl 2-trifluorobutynoate and substituted azides in terms of reactivity indices and activation parameters. Journal of Molecular Graphics and Modelling, 2017, 73, 143-151.	2.4	12
23	Ab initio study of the predissociation processes of the ground and first excited states of N2O+. Potential curves of the lowest states of N2O+. Computational and Theoretical Chemistry, 1994, 306, 313-320.	1.5	11
24	Electronic States of the Ultramarine Chromophore S3 -. Zeitschrift Fur Physikalische Chemie, 2008, 222, 163-176.	2.8	11
25	Accurate theoretical spectroscopy of the lowest electronic states of CP radical. Molecular Physics, 2014, 112, 2633-2645.	1.7	11
26	Theoretical spectroscopic characterization at low temperatures of methyl hydroperoxide and three S-analogs. Journal of Chemical Physics, 2015, 142, 074304.	3.0	11
27	Explicitly correlated interaction potential energy profile of imidazoleÂ+ÂCO2 complex. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	10
28	Unveiling the mechanism and selectivity of [3+2] cycloaddition reactions of benzonitrile oxide to ethyl trans-cinnamate, ethyl crotonate and trans-2-penten-1-ol through DFT analysis. Journal of Molecular Modeling, 2020, 26, 279.	1.8	10
29	RÃ©action hÃ©tÃ©ro-Dielsâ€“Alder nitrosoalcÃ¨nes avec le 2H-pyrrole approche expÃ©rimentale et thÃ©orique. Tetrahedron, 2002, 58, 1507-1512.	1.9	9
30	Ab-initio potential energy curves of valence and Rydberg electronic states of the PO radical. Computational and Theoretical Chemistry, 2014, 1049, 102-108.	2.5	9
31	Stability of Van der Waals complexes of the greenhouse effect gases CH4 and SF6 with imidazole in gas mixtures containing CO2. Computational and Theoretical Chemistry, 2016, 1094, 82-91.	2.5	9
32	On the Electronic States of S4+ and S4- Isomers. Collection of Czechoslovak Chemical Communications, 2007, 72, 83-99.	1.0	8
33	Influence of the functionalization of imidazole on its CO 2 uptake efficiency. A theoretical contribution. Computational and Theoretical Chemistry, 2015, 1073, 1-8.	2.5	8
34	Adsorption of imidazole on Au(111) surface: Dispersion corrected density functional study. Applied Surface Science, 2016, 383, 233-239.	6.1	8
35	Anti-corrosion performance of pyran-2-one derivatives for mild steel in acidic medium: Electrochemical and theoretical study. Chemical Data Collections, 2021, 32, 100655.	2.3	8
36	Low lying quartet states in diacetylene, triacetylene and benzene radical cations â€“ ARTICLE WITHDRAWN. Molecular Physics, 2006, 104, 3281-3285.	1.7	7

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37	Ab initiostudy of PN electronic states â€“ a qualitative interpretation of the perturbation and predissociation effects on observed transitions. Molecular Physics, 2014, 112, 117-126.	1.7	7
38	Theoretical study of the electron attachment dissociation of methyl halides and freon molecules: CF 3 Cl, CF 2 Cl 2 , CFCl 3. Journal of Fluorine Chemistry, 2001, 108, 177-186.	1.7	5
39	The spinâ€“orbit coupling in the bond formation region of the electronic ground states of , and. Chemical Physics, 2006, 329, 251-255.	1.9	5
40	A computational investigation on the adsorption of amoxycillin on graphene oxide nanosheet. International Journal of Environmental Analytical Chemistry, 0, , 1-9.	3.3	4
41	A representation of effective potentials of molecular fragments (NH3, PH3, AsH3): applications to AH3î—¸EH3 systems, where A is B, Al, Ga, In or Tl, and E is N, P or As. Computational and Theoretical Chemistry, 1995, 358, 219-228.	1.5	3
42	Approche thÃ©orique de la cycloaddition dipolaire-1,3 sur des dipolarophiles fluorÃ©s. Journal of Fluorine Chemistry, 1999, 94, 127-133.	1.7	3
43	Low lying quartet states in diacetylene, triacetylene and benzene radical cations. Molecular Physics, 2007, 105, 893-897.	1.7	3
44	Molecular structure and vibrational study of diprotonated guanazolium using DFT calculations and FT-IR and FT-Raman spectroscopies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 97, 975-985.	3.9	3
45	Spectral characteristics and DFT Study of vanadyl octaethylporphyrin complex. Mediterranean Journal of Chemistry, 2019, 8, 132-139.	0.7	3
46	Exploring QSAR of non-nucleoside reverse transcriptase inhibitors by artificial neural networks: HEPT derivatives. Arkivoc, 2007, 2007, 245-256.	0.5	3
47	Etude thÃ©orique de la dissociation de NO par attachement Ã©lectronique â€” courbes de potential ab initio de diffÃ©rents Ã©tats excitÃ©s de NOâ^. Computational and Theoretical Chemistry, 1993, 279, 7-14.	1.5	2
48	A theoretical investigation of the conformational aspects of aminophenols and of their complexation with BF 2 + and ZnCl 2. Computational and Theoretical Chemistry, 2000, 531, 223-239.	1.5	2
49	First-principle computations of rotational-vibrational transition probabilities. Molecular Physics, 2008, 106, 2001-2009.	1.7	2
50	On the formation of S2O at low energies: An ab initio study. Chemical Physics Letters, 2010, 500, 207-210.	2.6	2
51	Theoretical Study of Reaction Between Nitrilimine and 1,4 Oxazine 2 Carboxylate by MP2 and DFT Methods. Oriental Journal of Chemistry, 2018, 34, 2992-2997.	0.3	2
52	Inhibition efficiency and adsorption mechanism of 4-aminobenzoic acid for copper corrosion in nitric acid medium: a combined experimental and theoretical investigation. Structural Chemistry, 2021, 32, 2183-2198.	2.0	2
53	Etude theorique des spectres photoelectronique et ultraviolet de l'anion CNâ^. Computational and Theoretical Chemistry, 1991, 228, 11-17.	1.5	1
54	Stability of van der Waals complexes of the greenhouse effect gases NH3, SO2 and CO with imidazole in gas mixtures containing CO2. Computational and Theoretical Chemistry, 2017, 1099, 8-13.	2.5	1

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55	Theoretical spectroscopic study of acetyl (CH3CO), vinoxy (CH2CHO), and 1-methylvinoxy (CH3COCH2) radicals. Barrierless formation processes of acetone in the gas phase. Open Research Europe, 0, 1, 116.	2.0	1
56	Theoretical study of the electronic states of newly detected dications. Case of MgS2+ AND SiN2+. ChemistrySelect, 2017, 2, .	1.5	0
57	Theoretical Approach of the Adsorption of Herbicide Amitrole on the Soil using DFT Method. Oriental Journal of Chemistry, 2018, 34, 1240-1248.	0.3	0
58	Theoretical study of the solvent effects on electronic properties of 2(1H)-quinoxalinone derivatives. Mediterranean Journal of Chemistry, 2016, 5, 554-567.	0.7	0
59	The formation of interstellar organic molecules: H2C3O A DFT and ELF theoretical study. Mediterranean Journal of Chemistry, 2019, 9, 175-189.	0.7	0
60	Theoretical spectroscopic study of acetyl (CH3CO), vinoxy (CH2CHO), and 1-methylvinoxy (CH3COCH2) radicals. Barrierless formation processes of acetone in the gas phase. Open Research Europe, 0, 1, 116.	2.0	0