L Senthilkumar

List of Publications by Year in descending order

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79 papers	1,258 citations	430754 18 h-index	434063 31 g-index
80 all docs	80 docs citations	80 times ranked	1513 citing authors

#	Article	IF	Citations
1	Adsorption behaviour of reduced graphene oxide towards cationic and anionic dyes: Co-action of electrostatic and Ï€ â€“ Ï€ interactions. Materials Chemistry and Physics, 2017, 194, 243-252.	2.0	198
2	Calcium decorated and doped phosphorene for gas adsorption. Applied Surface Science, 2016, 377, 311-323.	3.1	80
3	Interaction studies of cysteine with Li⁺, Na⁺, K⁺, Be²⁺, Mg²⁺, and Ca²⁺metal cation complexes. Journal of Physical Organic Chemistry, 2011, 24, 553-567.	0.9	56
4	Hydrogen Bonding in Substituted Formic Acid Dimers. Journal of Physical Chemistry A, 2006, 110, 12623-12628.	1.1	48
5	Electron Density and Energy Decomposition Analysis in Hydrogen-Bonded Complexes of Azabenzenes with Water, Acetamide, and Thioacetamide. Journal of Physical Chemistry A, 2005, 109, 7575-7582.	1.1	44
6	Multiwalled Carbon Nanotube Oxygen Sensor: Enhanced Oxygen Sensitivity at Room Temperature and Mechanism of Sensing. ACS Applied Materials & Interfaces, 2015, 7, 23857-23865.	4.0	40
7	H, OH and COOH functionalized magnesium phthalocyanine as a catalyst for oxygen reduction reaction (ORR) â€“ A DFT study. International Journal of Hydrogen Energy, 2020, 45, 8540-8548.	3.8	34
8	Coordination and binding properties of zwitterionic glutathione with transition metal cations. Inorganica Chimica Acta, 2012, 387, 125-136.	1.2	30
9	Glutathione functionalized copper nanoclusters as a fluorescence platform for specific biosensing of cysteine and application in cellular imaging. Microchemical Journal, 2020, 158, 105253.	2.3	29
10	Theoretical studies on hydrogen bonding in caffeineâ€“theophylline complexes. Computational and Theoretical Chemistry, 2012, 979, 54-63.	1.1	27
11	Hydrogen-bonded complexes of serotonin with methanol and ethanol: a DFT study. Structural Chemistry, 2014, 25, 139-157.	1.0	27
12	Degradation of methyl salicylate through Cl initiated atmospheric oxidation â€“ a theoretical study. RSC Advances, 2014, 4, 23464.	1.7	26
13	Influence of in-plane Stoneâ€“Throwerâ€“Wales defects and edge functionalisation on the adsorption of CO2and H2O on graphene. RSC Advances, 2014, 4, 39576.	1.7	25
14	Interface energetics of [Emim] + [X] â^' and [Bmim] + [X] â^' (X = BF 4 , Cl, PF 6 , TfO, Tf 2 N) based ionic liquids on graphene, defective graphene, and graphyne surfaces. Journal of Molecular Liquids, 2017, 236, 124-134.	2.3	23
15	Theoretical investigations on the hydrogen bonding of nitrile isomers with H₂O, HF, NH₃and H₂S. Molecular Simulation, 2013, 39, 908-921.	0.9	22
16	DFT study on Xâ^'Â·(H2O)n=1-10 (X=OH, NO2, NO3, CO3) anionic water cluster. Journal of Molecular Graphics and Modelling, 2014, 54, 148-163.	1.3	22
17	Improved lithium adsorption in boron- and nitrogen-substituted graphene derivatives. Journal of Materials Science, 2017, 52, 815-831.	1.7	21
18	Cobalt phthalocyanine is a suitable scaffold for lithium polysulfide (Li2Sn nâ€¯=â€¯2â€“8). Chemical Physics Letters, 2020, 739, 136942.	1.2	20

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19	Study of effective hardness and condensed Fukui functions using AIM,ab initio, and DFT methods. Molecular Physics, 2005, 103, 547-556.	0.8	18
20	Pyrrolic, pyridinic, and graphitic sumanene as metalâ€free catalyst for oxygen reduction reaction â€“ A density functional theory study. Fuel Cells, 2021, 21, 490-501.	1.5	18
21	Hydrogen-bond interactions in hydrated 6-selenoguanine tautomers: a theoretical study. Structural Chemistry, 2014, 25, 197-213.	1.0	15
22	DFT study on abstraction reaction mechanism of oh radical with 2-methoxyphenol. Journal of Physical Organic Chemistry, 2017, 30, e3713.	0.9	15
23	Gas adsorption efficacy of graphene sheets functionalised with carboxyl, hydroxyl and epoxy groups in conjunction with Stoneâ€“Throwerâ€“Wales (STW) and inverse Stoneâ€“Throwerâ€“Wales (ISTW) defects. Physical Chemistry Chemical Physics, 2017, 19, 30895-30913.	1.3	15
24	Theoretical study on the interaction of CO₂ and H₂O molecules with metal doped-fluorinated phthalocyanines. New Journal of Chemistry, 2018, 42, 3465-3472.	1.4	15
25	Density functional theory investigation of cocaine water complexes. Journal of Molecular Modeling, 2013, 19, 3411-3425.	0.8	14
26	Edge functionalised & Li-intercalated 555-777 defective bilayer graphene for the adsorption of CO2 and H2O. Applied Surface Science, 2017, 400, 375-390.	3.1	14
27	Synthesis of metal-free nitrogen-enriched porous carbon and its electrochemical sensing behavior for the highly sensitive detection of dopamine: Both experimental and theoretical investigation. Materials Chemistry and Physics, 2021, 260, 124094.	2.0	14
28	Post Hartreeâ€“Fock and density functional theory studies on tautomerism of 6-thioxanthine in gas phase and in solution. Computational and Theoretical Chemistry, 2003, 638, 69-78.	1.5	13
29	Molecular interaction study of formohydroxamic acid (FHA) with water. Journal of Molecular Structure, 2006, 791, 149-157.	1.8	13
30	Defect-Mediated Reduction in Barrier for Helium Tunneling through Functionalized Graphene Nanopores. Journal of Physical Chemistry C, 2015, 119, 20940-20948.	1.5	13
31	DFT study of chemical reactivity parameters of lithium polysulfide molecules Li2Sn<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"><mml:mrow><mml:mo stretchy="false">(</mml:mo><mml:mn>1</mml:mn><mml:mo>â‰¤</mml:mo><mml:mi) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50	1.1	13
32	Theoretical Chemistry, 2021, 1202, 113323. Influence of metal ions (Zn²⁺, Cu²⁺, Ca²⁺, Mg²⁺and) Tj ETQq0 0 0 rgBT /Overlock Advances, 2014, 4, 49040-49052.	1.7	12
33	An experimental and theoretical study of the kinetics of the reaction between 3-hydroxy-3-methyl-2-butanone and OH radicals. RSC Advances, 2015, 5, 26559-26568.	1.7	12
34	Elucidation of Binding Mechanism of Photodynamic Therapeutic Agent Toluidine Blue O with Chicken Egg White Lysozyme by Spectroscopic and Molecular Dynamics Studies. Photochemistry and Photobiology, 2017, 93, 1043-1056.	1.3	12
35	Experimental and theoretical investigations of the kinetics and mechanism of the ClÂ+ 4-hydroxy-4-methyl-2-pentanone reaction. Atmospheric Environment, 2017, 166, 315-326.	1.9	12
36	Reaction of <scp>OH</scp> radical and ozone with methyl salicylate â€“ a <scp>DFT</scp> study. Journal of Physical Organic Chemistry, 2015, 28, 542-553.	0.9	11

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37	The influence of interfaces and intra-band transitions on the band gap of CdS/HgS and GaN/X (X=InN, In) Tj ETQq1 1 0.784314 rgBT /O Low-Dimensional Systems and Nanostructures, 2015, 74, 204-212.	1.3	10
38	Theoretical studies on interaction of anticancer drugs (dacarbazine, procarbazine and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 707 Td (trie Simulation, 2015, 41, 633-652.	0.9	10
39	Addition and abstraction reaction mechanism of 2,4,5-trimethylphenol with OH radical â€“ A first principle study. Computational and Theoretical Chemistry, 2016, 1092, 90-107.	1.1	10
40	Understanding molecular properties of halogenated cyclohexane â€“ A DFT study. Computational and Theoretical Chemistry, 2014, 1049, 55-61.	1.1	9
41	Atmospheric fate of diketones and OH radicalâ€“kinetics, reaction force, ETS-NOCV analysis. Molecular Physics, 2017, 115, 839-859.	0.8	9
42	Reaction of NO3 radical with benzyl alcohol - A DFT study. Computational and Theoretical Chemistry, 2017, 1102, 51-59.	1.1	9
43	Impact of functional groups substitution on the molecular properties of magnesium and scandium phthalocyanines. Inorganica Chimica Acta, 2018, 483, 203-210.	1.2	9
44	Hydrogenâ€bonded complexes of nicotine with simple alcohols. International Journal of Quantum Chemistry, 2012, 112, 2787-2793.	1.0	8
45	Structure and NLO properties of halogen (F, Cl) substituted formic acid dimers. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 132, 821-832.	2.0	8
46	DFT study on the tautomerism of organic linker 1H-imidazole-4,5-tetrazole (HIT). Computational and Theoretical Chemistry, 2015, 1068, 149-159.	1.1	8
47	Reaction of Pentanol isomers with OH radicalÂâ€“ÂA theoretical perspective. Molecular Physics, 2018, 116, 1153-1165.	0.8	8
48	Câ€“HÂ·Â·Â·O interaction between cation and anion in amino acid-based ionic liquidsâ€”A DFT study in gas and solvent phase. Structural Chemistry, 2019, 30, 185-194.	1.0	8
49	Chemical Properties of Lithium Cluster (Li_x, x = 2â€“8) on Stoneâ€“Wales Defect Graphene Sheet: A DFT Study. Journal of Physical Chemistry C, 2020, 124, 7229-7237.	1.5	8
50	Nitrogen-Doped Buckybowls as Potential Scaffold Material for Lithium-Sulfur Battery: A DFT Study. Electrocatalysis, 2021, 12, 678-690.	1.5	8
51	Spectroscopic investigations and hydrogen bond interactions of 8-aza analogues of xanthine, theophylline and caffeine: a theoretical study. Journal of Molecular Modeling, 2013, 19, 1835-1851.	0.8	7
52	Encapsulation of fluoroethanols in pristine and Stoneâ€“Wales defect boron nitride nanotube â€“ A DFT study. Applied Surface Science, 2015, 345, 369-378.	3.1	7
53	Theoretical investigations on hydrated 6,8-dithioguanine tautomers. Structural Chemistry, 2012, 23, 1203-1218.	1.0	6
54	Impact of heterogeneous passivation of trimethylphosphine oxide and di-methylphosphine oxide surface ligands on the electronic structure of Cd n Se n (n =6, 15) quantum dots: A DFT study. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 83, 284-296.	1.3	6

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55	First Experimental and Theoretical Kinetic Study of the Reaction of 4â€Hydroxyâ€4â€methyl 2â€pentanone as a Function of Temperature. International Journal of Chemical Kinetics, 2016, 48, 584-600.	1.0	6
56	OH initiated oxidation mechanism of monoterpene (linalool) â€“ A first comprehensive theoretical study. Atmospheric Environment, 2018, 189, 235-243.	1.9	6
57	Adsorption and sensing properties of non-planar ÏŒ surfaces towards high energy molecules: A density functional theory study. Journal of Physics and Chemistry of Solids, 2020, 138, 109198.	1.9	6
58	Photoactive amorphous molecular materials based on bisquinoline diamines and their synthesis by FriedlÃnder condensation reaction. Journal of Photochemistry and Photobiology A: Chemistry, 2014, 283, 45-55.	2.0	5
59	Metal-interacted histidine dimer: an ETS-NOCV and XANES study. RSC Advances, 2016, 6, 38919-38930.	1.7	5
60	Influence of dopants Cu, Ga, In, Hg on the electronic structure of Cd_nS_n (n =) Tj ETQq0 0 0 rgBT /Overlock 10	1.7	5
61	Hydrogen bonds in Zif268 proteins â€“ a theoretical perspective. Journal of Biomolecular Structure and Dynamics, 2016, 34, 1607-1624.	2.0	5
62	An experimental and theoretical study on the kinetics of the reaction between 4â€hydroxyâ€3â€hexanone CH₃CH₂C(O)CH(OH)CH₂CH₃ and OH radicals. International Journal of Chemical Kinetics, 2018, 50, 556-567.	1.0	5
63	Water confined (H2O) n=1â€“10 amino acid-based ionic liquids â€“ A DFT study on the bonding, energetics and IR spectra. Journal of Molecular Liquids, 2020, 304, 112720.	2.3	5
64	Complexes of criegee intermediate CH2OO with CO, CO2, H2O, SO2, NO2, CH3OH, HCOOH and CH3CH3CO molecules â€“ A DFT study on bonding, energetics and spectra. Computational and Theoretical Chemistry, 2021, 1203, 113341.	1.1	5
65	Facile Hydrothermal Synthesis and First Principle Computational Studies of NiSb₂O₄ and Its Electrochemical Properties with Ni₃(Fe(CN)₆)₂(H₂O) for Hybrid Supercapacitors. ChemistrySelect, 2017, 2, 6823-6832.	0.7	4
66	Effect of metal substitution (Mg, Sc) and functionalization (H, F, NH2, CH3, OH, CHO, and COOH) on the absorption properties of phthalocyanines â€“ A TDDFT study. Polyhedron, 2020, 176, 114244.	1.0	4
67	Cation-Anion Interactions, Stability, and IR Spectra of Dicationic Amino Acid-Based Ionic Liquids Probed Using Density Functional Theory. Journal of Molecular Modeling, 2021, 27, 180.	0.8	4
68	Enhancement of electrochemical performances of Li-S batteries using PPESK and Nelumbo nucifera derived porous carbon modified separator. Materials Letters, 2022, 315, 131935.	1.3	4
69	Importance of hydrogen bonding for second harmonic generation effect: X-ray diffraction and DFT study on S-benzyl isothiouronium chloride. Journal of Physics and Chemistry of Solids, 2009, 70, 322-325.	1.9	3
70	The study of performance of DFT functional for van der Waals interactions. Computational and Theoretical Chemistry, 2013, 1004, 56-60.	1.1	3
71	The first-principles study of CoSb2O4 and its electrochemical properties for supercapacitors. Electrochimica Acta, 2018, 283, 949-958.	2.6	3
72	Adsorption properties of amino acid-based ionic liquids (AAILs) on edge fluorinated graphene surface â€“ a DFT study. Molecular Simulation, 2021, 47, 1066-1077.	0.9	3

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73	Effect of alkyl chain on the NLO property of nonylphenol isomers: a DFT study. Monatshefte FÃ¼r Chemie, 2015, 146, 1983-1994.	0.9	2
74	ZnO and TiO₂ clusters as catalyst in the addition and abstraction reaction of acrylic acid with the OH radical. International Journal of Chemical Kinetics, 2020, 52, 3-15.	1.0	2
75	Theoretical perspective on the interaction of CO2 and H2O molecules with functionalized magnesium and scandium phthalocyanines. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	2
76	Molecular properties of metal difluorides and their interactions with CO2 and H2O molecules: a DFT investigation. Journal of Molecular Modeling, 2017, 23, 345.	0.8	1
77	Experimental and Theoretical Studies of Trans-2-Pentenal Atmospheric Ozonolysis. Atmosphere, 2022, 13, 291.	1.0	1
78	Study on the Iâ€“V characteristics of quantum well/dot embedded GaAs/AlGaAs structures - A transfer matrix method. AIP Conference Proceedings, 2015, , .	0.3	0
79	Interaction between arginine conformers and Hofmeister halide anions. Computational and Theoretical Chemistry, 2016, 1095, 93-103.	1.1	0