L Senthilkumar

List of Publications by Year in Descending Order

78 papers	897 citations	15 h-index	26 g-index
80 ext. papers	1,069 ext. citations	3.1 avg, IF	4.87 L-index

#	Paper	IF	Citations
78	Experimental and Theoretical Studies of Trans-2-Pentenal Atmospheric Ozonolysis. *Atmosphere*, **2022**, 13, 291	2.7	
77	Enhancement of electrochemical performances of Li-S batteries using PPESK and Nelumbo nucifera derived porous carbon modified separator. *Materials Letters*, **2022**, 315, 131935	3.3	
76	Pyrrolic, pyridinic, and graphitic sumanene as metal-free catalyst for oxygen reduction reaction A density functional theory study. *Fuel Cells*, **2021**, 21, 490	2.9	2
75	Theoretical perspective on the interaction of CO2 and H2O molecules with functionalized magnesium and scandium phthalocyanines. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9	0
74	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	2	2
73	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	4.4	4
72	Adsorption properties of amino acid-based ionic liquids (AAILs) on edge fluorinated graphene surface a DFT study. *Molecular Simulation*, **2021**, 47, 1066-1077	2	0
71	DFT study of chemical reactivity parameters of lithium polysulfide molecules Li2Sn(1 8) in gas and solvent phase. *Computational and Theoretical Chemistry*, **2021**, 1202, 113323	2	3
70	Nitrogen-Doped Buckybowls as Potential Scaffold Material for Lithium-Sulfur Battery: A DFT Study. *Electrocatalysis*, **2021**, 12, 678	2.7	1
69	Complexes of criegee intermediate CH2OO with CO, CO2, H2O, SO2, NO2, CH3OH, HCOOH and CH3CH3CO molecules A DFT study on bonding, energetics and spectra. *Computational and Theoretical Chemistry*, **2021**, 1203, 113341	2	0
68	Chemical Properties of Lithium Cluster (Lix, x = 2 8) on Stone Wales Defect Graphene Sheet: A DFT Study. *Journal of Physical Chemistry C*, **2020**, 124, 7229-7237	3.8	3
67	Glutathione functionalized copper nanoclusters as a fluorescence platform for specific biosensing of cysteine and application in cellular imaging. *Microchemical Journal*, **2020**, 158, 105253	4.8	10
66	Water confined (H2O) n=1 10 amino acid-based ionic liquids A DFT study on the bonding, energetics and IR spectra. *Journal of Molecular Liquids*, **2020**, 304, 112720	6	3
65	H, OH and COOH functionalized magnesium phthalocyanine as a catalyst for oxygen reduction reaction (ORR) A DFT study. *International Journal of Hydrogen Energy*, **2020**, 45, 8540-8548	6.7	11
64	Effect of metal substitution (Mg, Sc) and functionalization (H, F, NH2, CH3, OH, CHO, and COOH) on the absorption properties of phthalocyanines A TDDFT study. *Polyhedron*, **2020**, 176, 114244	2.7	0
63	Cobalt phthalocyanine is a suitable scaffold for lithium polysulfide (Li2Sn n = 2 8). *Chemical Physics Letters*, **2020**, 739, 136942	2.5	9
62	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	1.4	1

61	Adsorption and sensing properties of non-planar surfaces towards high energy molecules: A density functional theory study. *Journal of Physics and Chemistry of Solids*, **2020**, 138, 109198	3.9	3
60	CH O interaction between cation and anion in amino acid-based ionic liquids A DFT study in gas and solvent phase. *Structural Chemistry*, **2019**, 30, 185-194	1.8	4
59	Reaction of Pentanol isomers with OH radical A theoretical perspective. *Molecular Physics*, **2018**, 116, 1153-1165	1.7	3
58	Theoretical study on the interaction of CO2 and H2O molecules with metal doped-fluorinated phthalocyanines. *New Journal of Chemistry*, **2018**, 42, 3465-3472	3.6	10
57	Impact of functional groups substitution on the molecular properties of magnesium and scandium phthalocyanines. *Inorganica Chimica Acta*, **2018**, 483, 203-210	2.7	5
56	An experimental and theoretical study on the kinetics of the reaction between 4-hydroxy-3-hexanone CH3CH2C(O)CH(OH)CH2CH3 and OH radicals. *International Journal of Chemical Kinetics*, **2018**, 50, 556-567	1.4	2
55	OH initiated oxidation mechanism of monoterpene (linalool) A first comprehensive theoretical study. *Atmospheric Environment*, **2018**, 189, 235-243	5.3	3
54	The first-principles study of CoSb2O4 and its electrochemical properties for supercapacitors. *Electrochimica Acta*, **2018**, 283, 949-958	6.7	
53	Atmospheric fate of diketones and OH radical kinetics, reaction force, ETS-NOCV analysis. *Molecular Physics*, **2017**, 115, 839-859	1.7	6
52	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	3.6	9
51	DFT study on abstraction reaction mechanism of oh radical with 2-methoxyphenol. *Journal of Physical Organic Chemistry*, **2017**, 30, e3713	2.1	10
50	Adsorption behaviour of reduced graphene oxide towards cationic and anionic dyes: Co-action of electrostatic and interactions. *Materials Chemistry and Physics*, **2017**, 194, 243-252	4.4	145
49	Interface energetics of [Emim] + [X] and [Bmim] + [X] (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	6	17
48	Reaction of NO3 radical with benzyl alcohol - A DFT study. *Computational and Theoretical Chemistry*, **2017**, 1102, 51-59	2	6
47	Edge functionalised & Li-intercalated 555-777 defective bilayer graphene for the adsorption of CO 2 and H 2 O. *Applied Surface Science*, **2017**, 400, 375-390	6.7	12
46	Experimental and theoretical investigations of the kinetics and mechanism of the Cl + 4-hydroxy-4-methyl-2-pentanone reaction. *Atmospheric Environment*, **2017**, 166, 315-326	5.3	7
45	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	1.8	3
44	Molecular properties of metal difluorides and their interactions with CO and HO molecules: a DFT investigation. *Journal of Molecular Modeling*, **2017**, 23, 345	2	1

43	Gas adsorption efficacy of graphene sheets functionalised with carboxyl, hydroxyl and epoxy groups in conjunction with Stone-Thrower-Wales (STW) and inverse Stone-Thrower-Wales (ISTW) defects. *Physical Chemistry Chemical Physics*, **2017**, 19, 30895-30913	3.6	11
42	Improved lithium adsorption in boron- and nitrogen-substituted graphene derivatives. *Journal of Materials Science*, **2017**, 52, 815-831	4.3	16
41	Hydrogen bonds in Zif268 proteins - a theoretical perspective. *Journal of Biomolecular Structure and Dynamics*, **2016**, 34, 1607-24	3.6	1
40	Interaction between arginine conformers and Hofmeister halide anions. *Computational and Theoretical Chemistry*, **2016**, 1095, 93-103	2	
39	First Experimental and Theoretical Kinetic Study of the Reaction of 4-Hydroxy-4-methyl 2-pentanone as a Function of Temperature. *International Journal of Chemical Kinetics*, **2016**, 48, 584-600	1.4	4
38	Calcium decorated and doped phosphorene for gas adsorption. *Applied Surface Science*, **2016**, 377, 311-323	3.7	69
37	Metal-interacted histidine dimer: an ETS-NOCV and XANES study. *RSC Advances*, **2016**, 6, 38919-38930	3.7	4
36	Impact of heterogeneous passivation of trimethylphosphine oxide and di-methylphosphine oxide surface ligands on the electronic structure of CdnSen (n=6, 15) quantum dots: A DFT study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2016**, 83, 284-296	3	6
35	Influence of dopants Cu, Ga, In, Hg on the electronic structure of CdnSn (n = 6, 15) clusters – a DFT study. *RSC Advances*, **2016**, 6, 93056-93067	3.7	4
34	Addition and abstraction reaction mechanism of 2,4,5-trimethylphenol with OH radical – A first principle study. *Computational and Theoretical Chemistry*, **2016**, 1092, 90-107	2	6
33	DFT study on the tautomerism of organic linker 1H-imidazole-4,5-tetrazole (HIT). *Computational and Theoretical Chemistry*, **2015**, 1068, 149-159	2	6
32	The influence of interfaces and intra-band transitions on the band gap of CdS/HgS and GaN/X (X=InN, In0.33Ga0.67N) core/shell/shell quantum dot quantum well – A theoretical study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2015**, 74, 204-212	3	8
31	Encapsulation of fluoroethanols in pristine and Stone–Wales defect boron nitride nanotube – A DFT study. *Applied Surface Science*, **2015**, 345, 369-378	6.7	7
30	Multiwalled Carbon Nanotube Oxygen Sensor: Enhanced Oxygen Sensitivity at Room Temperature and Mechanism of Sensing. *ACS Applied Materials & Interfaces*, **2015**, 7, 23857-65	9.5	28
29	Defect-Mediated Reduction in Barrier for Helium Tunneling through Functionalized Graphene Nanopores. *Journal of Physical Chemistry C*, **2015**, 119, 20940-20948	3.8	13
28	Theoretical studies on interaction of anticancer drugs (dacarbazine, procarbazine and triethylenemelamine) with normal (AT and GC) and mismatch (GG, CC, AA and TT) base pairs. *Molecular Simulation*, **2015**, 41, 633-652	2	9
27	Reaction of OH radical and ozone with methyl salicylate – a DFT study. *Journal of Physical Organic Chemistry*, **2015**, 28, 542-553	2.1	9
26	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	3.7	11

25	Effect of alkyl chain on the NLO property of nonylphenol isomers: a DFT study. *Monatshefte Fü Chemie*, **2015**, 146, 1983-1994	1.4	2
24	DFT study on X?(HO)(n=1-10) (X=OH, NO, NO, CO) anionic water cluster. *Journal of Molecular Graphics and Modelling*, **2014**, 54, 148-63	2.8	18
23	Influence of in-plane Stone Thrower Wales defects and edge functionalisation on the adsorption of CO2 and H2O on graphene. *RSC Advances*, **2014**, 4, 39576	3.7	21
22	Degradation of methyl salicylate through Cl initiated atmospheric oxidation a theoretical study. *RSC Advances*, **2014**, 4, 23464	3.7	19
21	Influence of metal ions (Zn2+, Cu2+, Ca2+, Mg2+ and Na+) on the water coordinated neutral and zwitterionic L-histidine dimer. *RSC Advances*, **2014**, 4, 49040-49052	3.7	8
20	Understanding molecular properties of halogenated cyclohexane A DFT study. *Computational and Theoretical Chemistry*, **2014**, 1049, 55-61	2	7
19	Photoactive amorphous molecular materials based on bisquinoline diamines and their synthesis by Friedlder condensation reaction. *Journal of Photochemistry and Photobiology A: Chemistry*, **2014**, 283, 45-55	4.7	5
18	Structure and NLO properties of halogen (F, Cl) substituted formic acid dimers. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 132, 821-32	4.4	8
17	Hydrogen-bond interactions in hydrated 6-selenoguanine tautomers: a theoretical study. *Structural Chemistry*, **2014**, 25, 197-213	1.8	15
16	Hydrogen-bonded complexes of serotonin with methanol and ethanol: a DFT study. *Structural Chemistry*, **2014**, 25, 139-157	1.8	22
15	Density functional theory investigation of cocaine water complexes. *Journal of Molecular Modeling*, **2013**, 19, 3411-25	2	10
14	The study of performance of DFT functional for van der Waals interactions. *Computational and Theoretical Chemistry*, **2013**, 1004, 56-60	2	3
13	Spectroscopic investigations and hydrogen bond interactions of 8-aza analogues of xanthine, theophylline and caffeine: a theoretical study. *Journal of Molecular Modeling*, **2013**, 19, 1835-51	2	7
12	Theoretical investigations on the hydrogen bonding of nitrile isomers with H2O, HF, NH3 and H2S. *Molecular Simulation*, **2013**, 39, 908-921	2	15
11	Theoretical studies on hydrogen bonding in caffeine heophylline complexes. *Computational and Theoretical Chemistry*, **2012**, 979, 54-63	2	22
10	Hydrogen-bonded complexes of nicotine with simple alcohols. *International Journal of Quantum Chemistry*, **2012**, 112, 2787-2793	2.1	8
9	Theoretical investigations on hydrated 6,8-dithioguanine tautomers. *Structural Chemistry*, **2012**, 23, 1203-1218	1.8	6
8	Coordination and binding properties of zwitterionic glutathione with transition metal cations. *Inorganica Chimica Acta*, **2012**, 387, 125-136	2.7	22

7	Interaction studies of cysteine with Li+, Na+, K+, Be2+, Mg2+, and Ca2+ metal cation complexes. *Journal of Physical Organic Chemistry*, **2011**, 24, 553-567	2.1	46
6	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	3.9	3
5	Hydrogen bonding in substituted formic acid dimers. *Journal of Physical Chemistry A*, **2006**, 110, 12623-8	2.8	44
4	Molecular interaction study of formohydroxamic acid (FHA) with water. *Journal of Molecular Structure*, **2006**, 791, 149-157	3.4	12
3	Electron density and energy decomposition analysis in hydrogen-bonded complexes of azabenzenes with water, acetamide, and thioacetamide. *Journal of Physical Chemistry A*, **2005**, 109, 7575-82	2.8	41
2	Study of effective hardness and condensed Fukui functions using AIM, ab initio, and DFT methods. *Molecular Physics*, **2005**, 103, 547-556	1.7	14
1	Post Hartree-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		12