Chin-Hung Lai

List of Publications by Year
in descending order

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		236612	168136
85	2,891	25	53
papers	citations	h-index	g-index

86	86	86	3725
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Insights into the crystal structure of two newly synthesized quinoxalines derivatives as potent inhibitor for c-Jun N-terminal kinases. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2797-2814.	2.0	5
2	Multiple 3D- and 2D-quantitative structureâ€“activity relationship models (QSAR), theoretical study and molecular modeling to identify structural requirements of imidazopyridine analogues as anti-infective agents against tuberculosis. Structural Chemistry, 2022, 33, 679-694.	1.0	31
3	Performance of triazole derivatives as potential corrosion in-hibitors for mild steel in a strong phosphoric acid medium: Combining experimental and computational (DFT, MDs & QSAR) approaches. Journal of Molecular Structure, 2022, 1256, 132515.	1.8	18
4	A new synthetic route for the preparation of 2,2â€²,5â€²â€trimethylâ€7â€oxoâ€4,7â€dihydroâ€[6,7â€²â€bipyrazolo[1,5â€a]pyrimidine]â€3,3â€²â€dicarbonitrile, structural elucidation, Hirshfeld surface analysis, energy framework, density functional theory and molecular docking investigations. Journal of the Chinese Chemical Society, 2022, 69, 717-730.	0.8	3
5	Novel 3-chloro-6-nitro-1H-indazole derivatives as promising antileishmanial candidates: synthesis, biological activity, and molecular modelling studies. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 151-167.	2.5	4
6	Synthesis, crystal structure investigation and computational approach to discover potential hydrazide derivatives as a potent inhibitor of cyclooxygenaseâ€2 enzyme. Journal of Biochemical and Molecular Toxicology, 2022, , e23082.	1.4	3
7	Regiodivergent Synthesis of Methylene and Methyl Ring-Fused Isoquinolinones: Base-Promoted Isomerization of N-Allyl Amides. Journal of Organic Chemistry, 2022, 87, 5925-5937.	1.7	1
8	Synthesis, crystal structure, and a molecular modeling approach to identify effective antiviral hydrazide derivative against the main protease of SARS-CoV-2. Journal of Molecular Structure, 2022, 1265, 133391.	1.8	6
9	Unexpected synthesis of novel 2-pyrone derivatives: crystal structures, Hirshfeld surface analysis and computational studies. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4859-4877.	2.0	7
10	Exploring the twisted molecular configurations for tuning their optical and nonlinear optical response properties: A quantum chemical approach. Journal of Molecular Graphics and Modelling, 2021, 102, 107766.	1.3	14
11	Synthesis, spectroscopy, crystal structure, TGA/DTA study, DFT and molecular docking investigations of (E)-4-(4-methylbenzyl)-6-styrylpyridazin-3(2H)-one. Journal of Molecular Structure, 2021, 1228, 129435.	1.8	55
12	RBBP6 interactome: RBBP6 isoform 3/DWNN and Nek6 interaction is critical for cell cycle regulation and may play a role in carcinogenesis. Informatics in Medicine Unlocked, 2021, 23, 100522.	1.9	1
13	Copper(I)-Catalyzed Nitrile-Addition/N-Arylation Ring-Closure Cascade: Synthesis of 5,11-Dihydro-6H-indolo[3,2-c]quinolin-6-ones as Potent Topoisomerase-I Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 1435-1453.	2.9	17
14	Synthesis, X-ray, spectroscopic characterization, Hirshfeld surface analysis, DFT calculation and molecular docking investigations of a novel 7-phenyl-2,3,4,5-tetrahydro-1H-1,4- diazepin-5-one derivative. Journal of Molecular Structure, 2021, 1234, 130146.	1.8	3
15	Synthesis, Crystal structure, Hirshfeld surface Analysis and computational approach of new 2-methylbenzimidazo[1,2-a]pyrimidin-4(1H)-one. Journal of Molecular Structure, 2021, 1239, 130497.	1.8	10
16	Synthesis, Crystal Structure, DFT Calculations and Hirshfeld Surface Analysis of 5-Bromo-1-decyl-2,3-dihydro-1H- indolin-2-one. Journal of Chemical Crystallography, 2020, 50, 330-337.	0.5	1
17	Synergy of Ionic and Dipolar Effects by Molecular Design for pH Sensing beyond the Nernstian Limit. Advanced Science, 2020, 7, 1901001.	5.6	4
18	Synthesis and characterization of novel Cu (II) and Zn (II) complexes of 5-{[(2-Hydroxyethyl) sulfanyl] methyl}-8-hydroxyquinoline as effective acid corrosion inhibitor by experimental and computational testings. Chemical Physics Letters, 2020, 754, 137771.	1.2	50

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19	Palladium-Catalyzed Stereoselective Aza-Wackerâ€“Heck Cyclization: One-Pot Stepwise Strategy toward Tetracyclic Fused Heterocycles. Organic Letters, 2020, 22, 9337-9341.	2.4	14
20	Synthesis, spectroscopic characterization, crystal structure, DFT, molecular docking and inÂvitro antibacterial potential of novel quinoline derivatives. Journal of Molecular Structure, 2020, 1209, 127940.	1.8	40
21	Synthesis, Crystal Structure and Computational Investigation of New 4â€Phenylâ€decahydroâ€1Hâ€1,5â€benzodiazepinâ€2â€one as Potent Inhibitor of Muâ€opioid Receptor. ChemistrySelect, 2020, 5, 4601-4607.	0.7	7
22	Synthesis, anticancer evaluation inÂvitro, DFT, Hirshfeld surface analysis of some new 4-(1,3-benzothiazol-2-yl)-3-methyl-1-phenyl-4,5-dihydro-1H-pyrazol-5-one derivatives. Journal of Molecular Structure, 2019, 1198, 126910.	1.8	10
23	Synthesis, spectroscopic characterization, thermal, XRD crystal structure, the PLATON structural analysis, and theoretical studies of a new 1,2,4-triazolo-[1,5-a]pyrimidines derivatives. Journal of Molecular Structure, 2019, 1184, 12-24.	1.8	10
24	Nanostructured silver dendrites for photon-induced Cysteine dimerization. Scientific Reports, 2019, 9, 20174.	1.6	8
25	A systematic study of the effects of thionation in naphthalene dimide derivatives to tune their nonlinear optical properties. Journal of Molecular Graphics and Modelling, 2019, 87, 68-75.	1.3	13
26	Synthesis, crystal structure, DFT calculations and Hirshfeld surface analysis of 2-(1-decyl-2-oxoindolin-3-ylidene)propanedinitrile. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 21-25.	0.2	3
27	Crystal structure, DFT study and Hirshfeld surface analysis of 1-nonyl-2,3-dihydro-1H-indole-2,3-dione. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1140-1144.	0.2	2
28	Crystal structure, computational study and Hirshfeld surface analysis of ethyl (2S,3R)-3-(3-amino-1H-1,2,4-triazol-1-yl)-2-hydroxy-3-phenylpropanoate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1919-1924.	0.2	1
29	Synthesis, crystal structure, Hirshfeld surface analysis, and DFT calculations of new 1-[(1-benzyl-1H-1,2,3-triazol-4-yl)methyl]-6-methoxy-1H-benzimidazol-2(3H)-one. Chemical Data Collections, 2018, 17-18, 472-482.	1.1	10
30	Synthesis, Experimental and Density Functional Theory (DFT) Studies on Solubility of Camptothecin Derivatives. Molecules, 2018, 23, 3170.	1.7	9
31	Crystal structure, DFT calculations and Hirshfeld surface analysis of 3-(4-methylphenyl)-6-nitro-1H-indazole. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1857-1861.	0.2	2
32	Protecting-Group-Free Synthesis of 1-Phenylisoquinolin-4-ols: Thermal Cyclization of Methyl 2-[(Diphenylmethylidene)amino]acetates. Journal of Organic Chemistry, 2017, 82, 12849-12856.	1.7	2
33	A convenient synthesis of chiral 2-methylenebenzo[e][1,4]diazepin-5-ones via a one-pot reductive cyclodehydration with retention of chirality. Tetrahedron Letters, 2016, 57, 4842-4844.	0.7	6
34	A Comparison of the Lewis Basicity of Diamidocarbenes and Diaminocarbenes. Australian Journal of Chemistry, 2015, 68, 1084.	0.5	1
35	Computational study of unsaturated and saturated cyclic (alkyl) (amino) carbene borane complexes. Computational and Theoretical Chemistry, 2015, 1051, 17-23.	1.1	3
36	HSbXH (XÂ=ÂN, P, As, Sb, and Bi) isomers in the singlet and triplet states. A theoretical study. Journal of Organometallic Chemistry, 2014, 751, 379-389.	0.8	3

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37	A comparison of diamino- and diamidocarbenes toward dimerization. Journal of Molecular Modeling, 2013, 19, 4387-4394.	0.8	2
38	Computational comparison of the kinetic stabilities of diamino- and diamidocarbenes in the 1,2-H shift reaction. Journal of Molecular Modeling, 2013, 19, 2935-2944.	0.8	3
39	A theoretical study on the hydrogen adducts of diamidocarbenes and diaminocarbenes. Journal of Molecular Modeling, 2013, 19, 5523-5532.	0.8	2
40	Computational Study of Xe(OH)4, XeO(OH)3â€“, and XeO2(OH)22â€“. Journal of Physical Chemistry A, 2012, 116, 10397-10402.	1.1	2
41	Harvesting Highly Electronically Excited Energy to Triplet Manifolds: State-Dependent Intersystem Crossing Rate in Os(II) and Ag(I) Complexes. Journal of the American Chemical Society, 2012, 134, 7715-7724.	6.6	101
42	Excited-State Intramolecular Proton Transfer Molecules Bearing o-Hydroxy Analogues of Green Fluorescent Protein Chromophore. Journal of Organic Chemistry, 2011, 76, 8189-8202.	1.7	118
43	Mesomorphism and Luminescence Properties of Platinum(II) Complexes with Tris(alkoxy)phenylâ€Functionalized Pyridyl Pyrazolate Chelates. Chemistry - A European Journal, 2011, 17, 546-556.	1.7	71
44	A systematic study of the stabilities of cyclic boryl anions. Journal of Molecular Modeling, 2010, 16, 713-723.	0.8	6
45	A computational study on the capability of boraneâ€cyclic boryl anion adducts to act as hydrogen atom donors. Journal of Computational Chemistry, 2010, 31, 2258-2262.	1.5	10
46	Photoisomerization of a Maleonitrileâ€Type Salen Schiff Base and Its Application in Fineâ€Tuning Infinite Coordination Polymers. Chemistry - A European Journal, 2010, 16, 3770-3782.	1.7	15
47	Cyclometalated Platinum(II) Complexes of Lepidine-Based Ligands as Highly Efficient Electrophosphors. Organometallics, 2010, 29, 3912-3921.	1.1	67
48	Multifunctional Deepâ€Blue Emitter Comprising an Anthracene Core and Terminal Triphenylphosphine Oxide Groups. Advanced Functional Materials, 2009, 19, 560-566.	7.8	242
49	A New Series of Quadrupolar Type Twoâ€Photon Absorption Chromophores Bearing 11, 12â€Dibutoxydibenzo[a,c]â€phenazine Bridged Amines; Their Applications in Twoâ€Photon Fluorescence Imaging and Twoâ€Photon Photodynamic Therapy. Advanced Functional Materials, 2009, 19, 2388-2397.	7.8	133
50	A Bipolar Host Material Containing Triphenylamine and Diphenylphosphorylâ€Substituted Fluorene Units for Highly Efficient Blue Electrophosphorescence. Advanced Functional Materials, 2009, 19, 2834-2843.	7.8	196
51	Syntheses, Photophysics, and Application of Iridium(III) Phosphorescent Emitters for Highly Efficient, Longâ€Life Organic Lightâ€Emitting Diodes. Chemistry - an Asian Journal, 2009, 4, 742-753.	1.7	36
52	15-Crown-5 Functionalized Au Nanoparticles Synthesized via Single Molecule Exchange on Silica Nanoparticles: Its Application to Probe 15-Crown-5/K⁺/15-Crown-5 â€œSandwichesâ€• as Linking Mechanisms. Journal of Physical Chemistry C, 2009, 113, 1686-1693.	1.5	23
53	Dual Excited-State Intramolecular Proton Transfer Reaction in 3-Hydroxy-2-(pyridin-2-yl)-4H-chromen-4-one. Journal of Physical Chemistry A, 2009, 113, 205-214.	1.1	58
54	Neutral, panchromatic Ru(ii) terpyridine sensitizers bearing pyridine pyrazolate chelates with superior DSSC performance. Chemical Communications, 2009, , 5844.	2.2	96

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55	Dual Fluorescent Photochromic Colorants Bearing Pyrano[3,2-c]chromen-5-one Moiety. Journal of Physical Chemistry A, 2009, 113, 9321-9328.	1.1	16
56	A theoretical study of thermodynamics and kinetics of nitrosamines: a potential no carrier. Theoretical Chemistry Accounts, 2008, 119, 453-462.	0.5	3
57	The theoretical comparison between two model NO carriers, MeSNO and MeSeNO. Journal of Molecular Modeling, 2008, 14, 1-9.	0.8	7
58	Excitedâ€State Double Proton Transfer in Model Base Pairs: The Stepwise Reaction on the Heterodimer of 7â€Azaindole Analogues. ChemPhysChem, 2008, 9, 293-299.	1.0	34
59	Cyano Analogues of 7â€Azaindole: Probing Excitedâ€State Chargeâ€Coupled Proton Transfer Reactions in Protic Solvents. ChemPhysChem, 2008, 9, 2221-2229.	1.0	11
60	Theoretical characterizations of HAsXH (X = N, P, As, Sb, and Bi) isomers in the singlet and triplet states. Journal of Computational Chemistry, 2008, 29, 2487-2499.	1.5	14
61	2,3-Disubstituted Thiophene-Based Organic Dyes for Solar Cells. Chemistry of Materials, 2008, 20, 1830-1840.	3.2	401
62	Simple organic molecules bearing a 3,4-ethylenedioxythiophene linker for efficient dye-sensitized solar cells. Chemical Communications, 2008, , 5152.	2.2	195
63	A Computational Study on the Kinetic Stability of Cyclic Boryl Anions~!2007-12-13~!2008-05-13~!2008-06-11~!. The Open Chemical Physics Journal, 2008, 1, 51-61.	0.7	6
64	Synthesis, structure and electroluminescent properties of cyclometalated iridium complexes possessing sterically hindered ligands. Dalton Transactions, 2007, , 3025.	1.6	32
65	Novel Oxazabicycles as a New Class of Photochromic Colorants. Organic Letters, 2007, 9, 5287-5290.	2.4	22
66	Pyreno[2,1-b]pyrrole and Bis(pyreno[2,1-b]pyrrole) as Selective Chemosensors of Fluoride Ion:â€‰ A Mechanistic Study.. Journal of Organic Chemistry, 2007, 72, 5465-5465.	1.7	2
67	Pyreno[2,1-b]pyrrole and Bis(pyreno[2,1-b]pyrrole) as Selective Chemosensors of Fluoride Ion:Â A Mechanistic Study. Journal of Organic Chemistry, 2007, 72, 3537-3542.	1.7	106
68	New Family of Rutheniumâ€Dyeâ€Sensitized Nanocrystalline TiO₂ Solar Cells with a High Solarâ€Energyâ€Conversion Efficiency. Advanced Functional Materials, 2007, 17, 2964-2974.	7.8	67
69	Can an OH radical form a strong hydrogen bond? A theoretical comparison with H2O. Journal of Computational Chemistry, 2007, 28, 1357-1363.	1.5	21
70	Osmium Complexes with Tridentate 6-Pyrazol-3-yl 2,2â€²-Bipyridine Ligands: Coarse Tuning of Phosphorescence from the Red to the Near-Infrared Region. Chemistry - an Asian Journal, 2007, 2, 155-163.	1.7	25
71	Theoretical Investigation of Cheletroptic Decarbonylation Reactions. Journal of Chemical Theory and Computation, 2006, 2, 1078-1084.	2.3	26
72	Extensive spectral tuning of the proton transfer emission from 550 to 675 nm via a rational derivatization of 10-hydroxybenzo[h]quinoline. Chemical Communications, 2006, , 4395.	2.2	145

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73	Tuning Excited-State Electron Transfer from an Adiabatic to Nonadiabatic Type in Donorâ^'Bridgeâ^'Acceptor Systems and the Associated Energy-Transfer Process. Journal of Physical Chemistry A, 2006, 110, 12136-12144.	1.1	46
74	Femtosecond Spectroscopy and Dynamics of the Azulenylosquaric Dye, a Nearâ€infrared Nonfluorogenic Quencher. Journal of the Chinese Chemical Society, 2006, 53, 1275-1283.	0.8	0
75	Two-photon absorption chromophores with a tunable [2,2â€²]bithiophene core. Tetrahedron, 2006, 62, 8467-8473.	1.0	12
76	Isomerization reactions of RSNO (R=H, C n H2n+1 nâ‰ 4). Theoretical Chemistry Accounts, 2006, 117, 145-152.	0.5	15
77	Femtosecond Dynamics on 2-(2â€²-Hydroxy-4â€²-diethylaminophenyl)benzothiazole: Solvent Polarity in the Excited-State Proton Transfer. ChemPhysChem, 2006, 7, 1372-1381.	1.0	55
78	A Theoretical Study of Substituent Effects on Germaniumâ^'Phosphorus Triple Bonds. Journal of Physical Chemistry A, 2002, 106, 575-579.	1.1	7
79	Effects of First-Row Substituents on Siliconâ^'Phosphorus Triple Bonds. Inorganic Chemistry, 2002, 41, 1320-1322.	1.9	20
80	Theoretical Study of the Relative Stabilities of Arsasilenes and Arsasilynes. Organometallics, 2002, 21, 397-400.	1.1	6
81	Relative stability of multiple bonds between germanium and arsenic. A theoretical study. Polyhedron, 2002, 21, 579-585.	1.0	9
82	Electronic relaxation effect on sequential Î±-cleavage bond dissociation energy for carbonyl compounds and the heavy analogues. Chemical Physics Letters, 2002, 359, 355-359.	1.2	0
83	Theoretical study of triple bonds to germanium: relative stabilities of germanitriles and germaimines. Chemical Communications, 2001, , 1120-1121.	2.2	8
84	B3LYP and CCSD(T) Studies of the Mechanisms of Unimolecular Reactions of HXCS (X = H and F). Journal of Physical Chemistry A, 2001, 105, 6932-6937.	1.1	14
85	Structures, vibrational spectra, and relative energies of HXSiS (X = H, F, and Cl) isomers. International Journal of Quantum Chemistry, 2001, 82, 14-25.	1.0	8