Shyi-Long Lee

List of Publications by Year
in descending order

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125 papers	1,619 citations	394421 19 h-index	434195 31 g-index
127 all docs	127 docs citations	127 times ranked	1104 citing authors

#	Article	IF	Citations
1	Computing relative stabilities of metallofullerenes by Gibbs energy treatments. Theoretical Chemistry Accounts, 2007, 117, 315-322.	1.4	104
2	Multifractal scaling analysis of reactions over fractal surfaces. Surface Science, 1995, 325, 294-310.	1.9	72
3	Many-body interaction in glycineâ€“(water)3 complex using density functional theory method. Journal of Chemical Physics, 2004, 120, 170-174.	3.0	71
4	A computational study of microsolvation effect on ethylene glycol by density functional method. Journal of Chemical Physics, 2004, 120, 7464-7469.	3.0	52
5	A Fractal Approach to Adsorption on Heterogeneous Solid Surfaces. 1. The Relationship between Geometric and Energetic Surface Heterogeneities. Journal of Physical Chemistry B, 2001, 105, 10847-10856.	2.6	51
6	Computed structure and energetics of La@C60. International Journal of Quantum Chemistry, 2005, 104, 272-277.	2.0	47
7	Computations in Treating Fullerenes and Carbon Aggregates. Reviews in Computational Chemistry, 2007, , 1-62.	1.5	42
8	C80, C86, C88: Semiempirical and ab initio SCF calculations. International Journal of Quantum Chemistry, 1997, 63, 529-535.	2.0	35
9	Computational study of glycineâ€“(water)3 complex by density functional method. Chemical Physics, 2005, 310, 281-285.	1.9	34
10	Computed stabilities in metallofullerene series: Al@C₈₂, Sc@C₈₂, Y@C₈₂, and La@C₈₂. International Journal of Quantum Chemistry, 2011, 111, 2712-2718.	2.0	34
11	Theoretical investigation for the hydrogen bond interaction in THFâ€“water complex. Chemical Physics Letters, 2004, 386, 351-355.	2.6	32
12	Topological analysis of eigenvectors of the adjacency matrices in graph theory: The concept of internal connectivity. Chemical Physics Letters, 1987, 137, 279-284.	2.6	26
13	Rationally designed imidazole derivative as colorimetric and fluorometric sensor for selective, qualitative and quantitative cyanide ion detection in real time samples. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 234, 118212.	3.9	26
14	Multifractal analysis of growing surfaces. Applied Surface Science, 2004, 238, 513-517.	6.1	25
15	Hybrid DFT and hyper-GGA DFT studies of the CO adsorption on Pt nanoclusters: Effects of the cluster size and better CO LUMO description. Chemical Physics Letters, 2010, 492, 98-102.	2.6	24
16	Theoretical studies on nonlinear optical properties of formaldehyde oligomers byab initio and density functional theory methods. Journal of Computational Chemistry, 2005, 26, 1543-1564.	3.3	23
17	Semiempirical calculations of molecular polarizabilities and hyperpolarizabilities of polycyclic aromatic compounds. International Journal of Quantum Chemistry, 1992, 44, 773-784.	2.0	22
18	Density functional study of hydrogen-bonded acetonitrile-water complex. International Journal of Quantum Chemistry, 2005, 102, 106-111.	2.0	22

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19	Multifractal analysis of diffusion-limited reactions over surfaces of diffusion-limited aggregates. Chemical Physics Letters, 1993, 207, 220-226.	2.6	20
20	Multifractal scaling analysis of autopoisoning reactions over a rough surface. Journal of Physics A, 2003, 36, 3757-3772.	1.6	20
21	Hydrogen-bond interaction in 1:1 complexes of tetrahydrofuran with water, hydrogen fluoride, and ammonia: A theoretical study. Journal of Chemical Physics, 2005, 123, 044308.	3.0	20
22	Topological analysis of the eigenvectors of the adjacency matrices in graph theory: Degenerate case. Chemical Physics Letters, 1989, 157, 229-232.	2.6	19
23	Chemical signed graph theory. International Journal of Quantum Chemistry, 1994, 49, 639-648.	2.0	19
24	Effect of surface roughness on diffusion limited reactions, a multifractal scaling analysis. Chemical Physics Letters, 2002, 351, 341-348.	2.6	19
25	Microsolvation effect on alanine: a many-body interaction study using ab initio method. Computational and Theoretical Chemistry, 2004, 683, 115-119.	1.5	19
26	Intermolecular orbital repulsion effect on the blue-shifted hydrogen bond. Chemical Physics Letters, 2005, 406, 143-147.	2.6	18
27	Computed structures and relative stabilities of Be@C74. International Journal of Quantum Chemistry, 2007, 107, 2494-2498.	2.0	18
28	Effect of microsolvation on zwitterionic glycine: an ab initio and density functional theory study. Journal of Molecular Modeling, 2008, 14, 385-392.	1.8	17
29	Highly Selective and Sensitive Colorimetric and Fluorimetric Sensor for Cu2+. Journal of Fluorescence, 2020, 30, 3-10.	2.5	17
30	Excited electronic states and relative stabilities of C80 isomers. International Journal of Quantum Chemistry, 2006, 106, 2222-2228.	2.0	16
31	Computations on three isomers of La@C₇₄. International Journal of Quantum Chemistry, 2008, 108, 2636-2640.	2.0	16
32	Intramolecular hydroarylation of aryl propargyl ethers catalyzed by indium: the mechanism of the reaction and identifying the catalytic species. Organic and Biomolecular Chemistry, 2016, 14, 6508-6516.	2.8	16
33	Eco-Friendly Sustainable Poly(benzoxazine-co-urethane) with Room-Temperature-Assisted Self-Healing Based on Supramolecular Interactions. ACS Omega, 2020, 5, 33178-33185.	3.5	16
34	Quantum Mechanical Calculations for the Misincorporation of Nucleotides Opposite Mutagenic 3,N⁴-Ethenocytosine. Journal of Physical Chemistry B, 2012, 116, 11173-11179.	2.6	15
35	Atomistic simulation on flavonoids derivatives as potential inhibitors of bacterial gyrase of Staphylococcus aureus. Journal of Biomolecular Structure and Dynamics, 2020, , 1-14.	3.5	15
36	Eigenvector and eigenvalues of some special graphs. IV. Multilevel circulants. International Journal of Quantum Chemistry, 1992, 41, 105-116.	2.0	14

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37	Multifractal scaling analysis of autocatalytic and autopoisoning reactions over DLA surfaces. Chemical Physics Letters, 1994, 228, 539-546.	2.6	14
38	Quantum Chemical AM1 Study of Growth Mechanisms of Fullerenes:Â A Facile C2Insertion Technique. Journal of Physical Chemistry B, 1999, 103, 3151-3155.	2.6	14
39	Hydrogen bonding interaction in sarcosine-water complex using ab initio and DFT method. International Journal of Quantum Chemistry, 2005, 101, 97-103.	2.0	14
40	Calculated relative yields for Sc2S@C82 and Y2S@C82. Theoretical Chemistry Accounts, 2011, 130, 549-554.	1.4	14
41	Quantum mechanistic insights on aryl propargyl ether Claisen rearrangement. Organic and Biomolecular Chemistry, 2014, 12, 4163-4171.	2.8	14
42	Topological analysis of eigenvalues of particle in one- and two-dimensional simple quantal systems: Net sign approach. International Journal of Quantum Chemistry, 1991, 39, 59-70.	2.0	13
43	A Comparative Study of C60, Si60, and Ge60. Fullerenes, Nanotubes, and Carbon Nanostructures, 1994, 2, 459-469.	0.6	13
44	Lattice model studies of CO oxidation kinetic oscillation over nano-scaled Pt particle: Effect of temperature variation and diffusion. Applied Surface Science, 2005, 252, 784-792.	6.1	13
45	Topological analysis of some special of graphs. Hypercubes. Chemical Physics Letters, 1990, 171, 385-388.	2.6	12
46	Growth mechanism of C28 (Td) fullerene: energetics and transition-state structures analysis. Chemical Physics Letters, 1999, 313, 437-444.	2.6	12
47	Quantum-Chemical Calculations of Model Systems of Interest in Fullerene-Based Superconductivity. Journal of Low Temperature Physics, 2003, 131, 1259-1263.	1.4	12
48	Understanding the Mechanism of S N 2â€² vs . S N 2 in Cascade Reaction of Î²â€Naphthol and Nitrostyrene Derived MBH Acetates. ChemistrySelect, 2020, 5, 3080-3084.	1.5	12
49	Topological analysis of five-vertex clusters of group IVA elements. Theoretica Chimica Acta, 1992, 81, 185-199.	0.8	11
50	Theoretical studies of the fullerene growth mechanism: Ring-collapse model to C28 and cascade bond formation. Journal of Chemical Physics, 2000, 112, 6355-6364.	3.0	11
51	C28 (D2): Fullerene growth mechanism. International Journal of Quantum Chemistry, 2001, 84, 642-648.	2.0	11
52	Net-sign identity information index: A novel approach towards numerical characterization of chemical signed graph theory. Chemical Physics Letters, 2008, 454, 133-138.	2.6	11
53	Stability calculations for Eu@C₇₄ isomers. International Journal of Quantum Chemistry, 2013, 113, 729-733.	2.0	11
54	Calculated Temperature Development of the Relative Stabilities of Yb@C82 Isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 147-154.	2.1	11

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55	The first highly selective turn â€œONâ€•fluorescent sensor for vanadyl (VO²⁺) ions: DFT studies and molecular logic gate behavior. New Journal of Chemistry, 2018, 42, 3833-3839.	2.8	11
56	Theoretical study of 3d-metal mononitrides using DFT method. International Journal of Quantum Chemistry, 2007, 107, 212-218.	2.0	10
57	Net signs and eigenvalues of molecular graphs: some analogies. Chemical Physics Letters, 1992, 191, 87-91.	2.6	9
58	The Mean Isomer Degeneracy of the Wiener Index. Journal of the Chinese Chemical Society, 1993, 40, 195-198.	1.4	9
59	Theoretical studies of the molecular second-order hyperpolarizabilities of polycyclic aromatics. International Journal of Quantum Chemistry, 1995, 56, 509-522.	2.0	9
60	Interaction of Adenine Adducts with Thymine:Â A Computational Study. Journal of Physical Chemistry B, 2007, 111, 2991-2998.	2.6	9
61	Hydrogen-bond interactions in THFâ€“H2Oâ€“HF: A theoretical study. International Journal of Quantum Chemistry, 2007, 107, 2015-2023.	2.0	9
62	Theoretical Study of Local Electronic Alloy Effects of OOH, OH, and O Adsorption on Ptâ€“Pd Cluster Model. Journal of Physical Chemistry C, 2011, 115, 9105-9116.	3.1	9
63	Mechanisms of metal-catalyzed cycloisomerizations of o-propargylbiaryls and o-allenylbiaryls to phenanthrenes: a DFT study. Catalysis Science and Technology, 2017, 7, 6026-6041.	4.1	9
64	Impact and Shear Behavior of PLA/12%Cu Reinforced Composite Filament Printed at Different FDM Conditions. Arabian Journal for Science and Engineering, 2021, 46, 12709-12720.	3.0	9
65	Simulation of diffusion-limited aggregation and reactions over its surfaces. International Journal of Quantum Chemistry, 1994, 52, 339-352.	2.0	8
66	Computational studies of less common fullerene-related species. International Journal of Quantum Chemistry, 1996, 60, 1567-1576.	2.0	8
67	Density functional theory study of contribution of many-body energies to binding energy for alanine-(water)4 complex. International Journal of Quantum Chemistry, 2005, 102, 174-177.	2.0	8
68	Model Calculations for the Misincorporation of Nucleotides Opposite Five-Membered Exocyclic DNA Adduct: N²,3-Ethenoguanine. Journal of Physical Chemistry B, 2011, 115, 10537-10546.	2.6	8
69	The role of cesium fluoride in aryl propargyl ether Claisen rearrangement and its mechanistic elucidation: a theoretical study. Structural Chemistry, 2016, 27, 1383-1393.	2.0	8
70	2A + B2 â†’2AB catalytic reaction over rough surface: the effect of Eley-Rideal mechanism. Catalysis Today, 2004, 97, 89-92.	4.4	7
71	Kinetic oscillation of carbon monoxide oxidation over nano-scaled catalyst involving temperature variation. Chemical Physics Letters, 2004, 400, 245-252.	2.6	7
72	Theoretical studies of growth mechanism of small fullerene cage C24 (D6d)+. International Journal of Quantum Chemistry, 2005, 103, 355-368.	2.0	7

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73	Computations of production yields for Ba@C₇₄ and Yb@C₇₄. Molecular Simulation, 2007, 33, 563-568.	2.0	7
74	Computational screening of metallofullerenes for nanoscience: Sr@C₇₄. Molecular Simulation, 2008, 34, 17-21.	2.0	7
75	The B3LYP and BMK studies of CO adsorption on Pt(1 1 1): An insight through the chemical bonding analysis. Chemical Physics Letters, 2012, 530, 64-70.	2.6	7
76	Towards Relative Populations of Non-Isomeric Metallofullerenes: La@C76( ) vs. La2@C76(,17490). Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 299-306.	2.1	7
77	Comment on â€˜Topological Analysis of the Eigenvalues of the Adjacency Matrices in Graph Theory: A Difficulty with the Concept of Internal Connectivityâ€™. Journal of the Chinese Chemical Society, 1989, 36, 63-65.	1.4	6
78	AM1 Computations of C60O2. Fullerenes, Nanotubes, and Carbon Nanostructures, 1994, 2, 73-88.	0.6	6
79	Heterogeneous reactions over fractal surfaces: A multifractal scaling analysis. International Journal of Quantum Chemistry, 1997, 64, 337-350.	2.0	6
80	Density functional theory study of formaldehyde oligomers. International Journal of Quantum Chemistry, 2005, 101, 67-72.	2.0	6
81	Interaction of Serotonin and Fluoxetine: Toward Understanding the Importance of the Chirality of Fluoxetine (S form and R form). Journal of Physical Chemistry B, 2009, 113, 14529-14535.	2.6	6
82	MICROHYDRATION OF HYDRONIUM ION AND ZÃœNDEL ION: A MANY-BODY ANALYSIS APPROACH. Journal of Theoretical and Computational Chemistry, 2010, 09, 177-187.	1.8	6
83	Net signs of molecular graphs: Dependence of molecular structure. International Journal of Quantum Chemistry, 1994, 49, 87-95.	2.0	5
84	Computations of the catalytic effects in the stone-wales fullerene isomerizations: N and CN agents. International Journal of Quantum Chemistry, 2004, 99, 634-639.	2.0	5
85	Many-body interactions of carbon monoxide cyclic oligomers: A computational study. International Journal of Quantum Chemistry, 2005, 103, 314-321.	2.0	5
86	Computational investigation on microsolvation of the osmolyte glycine betaine [GB (H2O)1-7]. Journal of Molecular Modeling, 2012, 18, 5017-5028.	1.8	5
87	Spectroscopic probe on Nâ€“Hâ‹¯N, Nâ€“Hâ‹¯O and controversial Câ€“Hâ‹¯O contact in Aâ€“T base pair: A DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 542-547.	3.9	5
88	Computations on Metallofullerenes Derivatized during Extraction: La@C80-C6H3Cl2 and La@C82-C6H3Cl2. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 173-181.	2.1	5
89	Density Functional Theory Study on the Mechanisms of Platinumâ€•and Goldâ€Catalyzed Cycloisomerizations of Biaryl Propargyl Alcohol and Indolyl Allenol to Phenanthrene and Carbazole. ChemistrySelect, 2018, 3, 12093-12107.	1.5	5
90	Eleyâ€“Rideal diffusion limited reactions over rough surface. Physical Chemistry Chemical Physics, 2002, 4, 5330-5334.	2.8	4

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91	Dynamic scaling of diffusion-limited reactions over fractal surfaces: computer simulation. Applied Surface Science, 2002, 196, 375-382.	6.1	4
92	Calibration of Relativistic Energyâ€Consistent Smallâ€Core Pseudopotentials for 3dâ€Transition Metals. Journal of the Chinese Chemical Society, 2003, 50, 583-592.	1.4	4
93	Novel information theoretic topological index Ik for unsaturated hydrocarbons. Chemical Physics Letters, 2004, 396, 465-468.	2.6	4
94	Autopoisoning reactions over rough surface: A multifractal scaling analysis. International Journal of Chemical Kinetics, 2005, 37, 175-182.	1.6	4
95	Stability Computations for Fullerenes and Metallofullerenes. World Scientific Series on Carbon Nanoscience, 2012, , 381-429.	0.1	4
96	Development of Optical Biosensor for the Detection of Glutamine in Human Biofluids Using Merocyanine Dye. Journal of Fluorescence, 2022, 32, 1389-1396.	2.5	4
97	Effective Detection of Phenylalanine Using Pyridine Based Sensor. Journal of Fluorescence, 2022, 32, 1481-1488.	2.5	4
98	Substituent Effects on the Chemical Reactivities of Tricarbonyl and Tetracarbonyl Iron Complexes of 7â€Azanorbornadiene Derivatives. Journal of the Chinese Chemical Society, 1993, 40, 503-507.	1.4	3
99	A Multifractal Approach to Heterogeneous Reactions over Fractal Surfaces. Journal of the Chinese Chemical Society, 1994, 41, 665-672.	1.4	3
100	Eleyâ€“Rideal reactions over rough surface: effect of sticking probability. Chemical Physics, 2005, 309, 103-107.	1.9	3
101	The failure of UMP2 on the ketoâ€“enol tautomerization of Î²-radical compounds: The effect of spin contamination. Chemical Physics Letters, 2013, 565, 18-21.	2.6	3
102	Correlation between substituent constants and hyperpolarizabilities for di-substituted trans-azobenzenes. Journal of Molecular Modeling, 2013, 19, 529-538.	1.8	3
103	Sm@C74: Computed Relative Isomeric Populations. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 235-242.	2.1	3
104	A chemodosimeter for selective fluorogenic and chromogenic detection of phenylenediamine isomers. Journal of the Iranian Chemical Society, 2022, 19, 2719-2726.	2.2	3
105	C61H2Fulleroid: AM1 Computational Study. Fullerenes, Nanotubes, and Carbon Nanostructures, 1994, 2, 13-24.	0.6	2
106	Thermal Interchanges in the Relative Stabilities of the C₆₀Ge Specles. Journal of the Chinese Chemical Society, 1994, 41, 635-638.	1.4	2
107	Conversion of edge-to-loop and loop-to-edge technique used to study [?2+?2] and [?2+?4] chemical reactions. International Journal of Quantum Chemistry, 1999, 75, 821-827.	2.0	2
108	Quantum Chemical AM1 Treatment of the Circumscribing Algorithm:â€‰ Fullerene Growth Mechanism. Journal of Chemical Information and Computer Sciences, 1999, 39, 1090-1093.	2.8	2

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109	A comparative study of the static third-order polarizabilities of bowl/non-cage to cage structures: a structure-property correlation study. Molecular Physics, 1999, 97, 987-991.	1.7	2
110	Nonlinear optical study of the five IPR isomers of C78 generated by capping C72 through C6. International Journal of Quantum Chemistry, 2000, 77, 574-579.	2.0	2
111	C60(NO2)2: Quantum-Chemical Evaluations of Structure, Energetics, and Vibrational Spectra. Fullerenes, Nanotubes, and Carbon Nanostructures, 2000, 8, 351-367.	0.6	2
112	Computational Studies of the Growth Mechanism of Small Fullerenes: A Ringâ€Stacking Model. Journal of the Chinese Chemical Society, 2003, 50, 575-582.	1.4	2
113	The first stacking-step in the kinetic-ring stacking mechanism of small fullerene growth. Chemical Physics Letters, 2004, 393, 222-227.	2.6	2
114	Computer Simulation of Eleyâ€Rideal Reactions Over Rough Surface. Journal of the Chinese Chemical Society, 2007, 54, 1201-1210.	1.4	2
115	Model calculations for the base-pairing specificity of mutagenic exocyclic DNA adduct 1,N 6-ethenoadenine. Structural Chemistry, 2014, 25, 561-573.	2.0	2
116	Effects of Microsolvation on the Electronic Properties of Sarcosine: A Computational Study. ChemistrySelect, 2017, 2, 8950-8958.	1.5	2
117	On the misincorporation of nucleotides opposite mutagenic cyclic 1,N2-propanoguanine: A computational investigation. Journal of Molecular Graphics and Modelling, 2018, 85, 270-280.	2.4	2
118	Structural effects on the low cubic hyperpolarizability of C60: A scaling of conjugation in three-dimensional curvature of ?-conjugation systems. International Journal of Quantum Chemistry, 1999, 75, 457-463.	2.0	1
119	Synchronization between Kinetic Oscillations Occurring on Neighboring Nanoscaled Supported Platinum Clusters via Thermal Conduction. Journal of Physical Chemistry C, 2009, 113, 5206-5211.	3.1	1
120	Structural and bonding features of Z@C82 (Z=Al, Sc, Y, La) endohedrals. Journal of Computational Methods in Sciences and Engineering, 2010, 10, 569-574.	0.2	1
121	Dynamic scaling for Eley-Rideal reactions over rough surface. International Journal of Chemical Kinetics, 2004, 36, 286-292.	1.6	0
122	Alkali-metal clusters encapsulated into fullerenes: Computations on Lix@C60. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 541-547.	0.2	0
123	Counterion Effect on the Mechanism of Gold(I)â€Catalyzed Cycloisomerization of 3â€Allenylmethylindoles to 4,9â€Dihydroâ€1 H â€Carbazoles: A Computational Study. ChemistrySelect, 2021, 6, 7482-7488.	1.5	0
124	On the Development and Application of Net-Sign Graph Theory. , 2011, , 127-151.		0
125	An Evaluation of Density Functional Theory for CO Adsorption on Pt(111). Progress in Theoretical Chemistry and Physics, 2013, , 195-210.	0.2	0