

# Feng Wang

## List of Publications by Year in descending order

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279  
papers

6,543  
citations

87843

38  
h-index

95218

68  
g-index

284  
all docs

284  
docs citations

284  
times ranked

6618  
citing authors

#	ARTICLE	IF	CITATIONS
1	Dibenzothiophene-S,S-dioxide-containing conjugated polymer with hydrogen evolution rate up to $147 \text{ } \mu\text{mol} \text{ } \text{h}^{-1} \text{ cm}^{-2}$ . Applied Catalysis B: Environmental, 2022, 307, 121144.	10.8	40
2	NMR Chemical Shift and Methylation of 4-Nitroimidazole: Experiment and Theory. Australian Journal of Chemistry, 2021, 74, 48.	0.5	2
3	Double transition metal atoms anchored on Graphdiyne as promising catalyst for electrochemical nitrogen reduction reaction. Journal of Materials Science and Technology, 2021, 77, 244-251.	5.6	63
4	Synthesis and characterisation of monolithic $\text{Pt}/\text{MnO}_x/\text{FeO}_x$ catalysts for selective catalytic reduction (SCR) of $\text{NO}_x$ at low temperature. Journal of Chemical Technology and Biotechnology, 2021, 96, 1016-1029.	1.6	5
5	Robust design of D-A model compounds using digital structures for organic DSSC applications. Journal of Molecular Graphics and Modelling, 2021, 102, 107798.	1.3	4
6	Realizing high hydrogen evolution activity under visible light using narrow band gap organic photocatalysts. Chemical Science, 2021, 12, 1796-1802.	3.7	77
7	Red-Edge Excitation Shift Spectroscopy (REES): Application to Hidden Bound States of Ligands in Protein-Ligand Complexes. International Journal of Molecular Sciences, 2021, 22, 2582.	1.8	6
8	Boosting the Photocatalytic Hydrogen Evolution Activity for $\text{D}^{\text{A}}$ Conjugated Microporous Polymers by Statistical Copolymerization. Advanced Materials, 2021, 33, e2008498.	11.1	143
9	Accelerating optical reporting for conformation of tyrosine kinase inhibitors in solutions. International Journal of Quantum Chemistry, 2021, 121, e26765.	1.0	6
10	Eliminating the Detrimental Effect of Secondary Doping on PEDOT:PSS Hole Transporting Material Performance. ChemSusChem, 2021, 14, 4802-4811.	3.6	5
11	A Case Study on a Soluble Dibenzothiophene-S,S-dioxide-Based Conjugated Polyelectrolyte for Photocatalytic Hydrogen Production: The Film versus the Bulk Material. ACS Applied Materials & Interfaces, 2021, 13, 42753-42762.	4.0	14
12	Dominance of eclipsed ferrocene conformer in solutions revealed by the IR spectra between 400 and 500 $\text{cm}^{-1}$ . Radiation Physics and Chemistry, 2021, 188, 109590.	1.4	2
13	Solvent contribution to ferrocene conformation: Theory and experiment. Radiation Physics and Chemistry, 2021, 189, 109697.	1.4	4
14	Differentiation of alkyl radicals: A route through chemical graph theory. International Journal of Quantum Chemistry, 2021, 121, e26567.	1.0	1
15	Positional and Conformational Isomerism in Hydroxybenzoic Acid: A Core-Level Study and Comparison with Phenol and Benzoic Acid. Journal of Physical Chemistry A, 2021, 125, 9877-9891.	1.1	6
16	Mechanistic Insights into Direct Methane Oxidation to Methanol on Single-Atom Transition-Metal-Modified Graphyne. ACS Applied Nano Materials, 2021, 4, 12006-12016.	2.4	17
17	Investigation of adsorption, dissociation, and diffusion properties of hydrogen on the V ( $11\bar{0}0$ ) surface and in the bulk: A first-principles calculation. Journal of Advanced Research, 2020, 21, 25-34.	4.4	14
18	Poly(dibenzothiophene-S,S-dioxide) with visible light-induced hydrogen evolution rate up to $44.2 \text{ } \mu\text{mol} \text{ } \text{h}^{-1} \text{ cm}^{-2}$ promoted by $\text{K}_2\text{HPO}_4$ . Applied Catalysis B: Environmental, 2020, 261, 118230.	10.8	40

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19	Substituent effect of conjugated microporous polymers on the photocatalytic hydrogen evolution activity. <i>Journal of Materials Chemistry A</i> , 2020, 8, 2404-2411.	5.2	91
20	Bisulfone- $\epsilon$ -Functionalized Organic Polymer Photocatalysts for High-Performance Hydrogen Evolution. <i>ChemSusChem</i> , 2020, 13, 369-375.	3.6	20
21	Impact of intramolecular hydrogen bonding of gallic acid conformers on chemical shift through NMR spectroscopy. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 95, 107486.	1.3	6
22	The electronic structure of bicyclo[2.2.2]octa-2,5-dione. <i>Chemical Physics Letters</i> , 2020, 757, 137877.	1.2	0
23	An experimental and theoretical investigation of XPS and NEXAFS of nicotine, nicotinamide, and nicotinic acid. <i>Journal of Physics: Conference Series</i> , 2020, 1412, 102008.	0.3	1
24	Cover Image, Volume 120, Issue 23. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26513.	1.0	0
25	The importance of the molecular weight of PEDOT hole transporting materials for efficient organic solar cells. <i>Journal of Materials Chemistry C</i> , 2020, 8, 17185-17193.	2.7	14
26	A high performance and low cost poly(dibenzothiophene- <i>S,S</i> -dioxide)@TiO <sub>2</sub> composite with hydrogen evolution rate up to 51.5 mmol h <sup>-1</sup> g <sup>-1</sup> . <i>Journal of Materials Chemistry A</i> , 2020, 8, 18292-18301.	5.2	23
27	Deducing the Conformational Properties of a Tyrosine Kinase Inhibitor in Solution by Optical Spectroscopy and Computational Chemistry. <i>Frontiers in Chemistry</i> , 2020, 8, 596.	1.8	4
28	Molecular dynamics study of ferrocene topology under various temperatures. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26398.	1.0	4
29	Theoretical Investigation of Single and Double Transition Metals Anchored on Graphyne Monolayer for Nitrogen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2020, 124, 15295-15301.	1.5	79
30	Structure evolution of azo-fused conjugated microporous polymers for high performance lithium-ion batteries anodes. <i>Journal of Power Sources</i> , 2020, 453, 227868.	4.0	30
31	Theoretical investigation of molybdenum/tungsten-vanadium solid solution alloy membranes: Thermodynamic stability and hydrogen permeation. <i>Journal of Membrane Science</i> , 2020, 608, 118200.	4.1	26
32	Resolution of ferrocene and deuterated ferrocene conformations using dynamic vibrational spectroscopy: Experiment and theory. <i>Inorganica Chimica Acta</i> , 2020, 506, 119491.	1.2	5
33	Thiophene-rich conjugated microporous polymers as anode materials for high performance lithium- and sodium-ion batteries. <i>Solid State Ionics</i> , 2020, 347, 115247.	1.3	18
34	Experimental and Theoretical Soft X-ray Study of Nicotine and Related Compounds. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4025-4035.	1.1	6
35	Switching On/Off the Intramolecular Hydrogen Bonding of 2-Methoxyphenol Conformers: An NMR Study. <i>Australian Journal of Chemistry</i> , 2020, 73, 222.	0.5	4
36	Probing Intramolecular Interaction of Stereoisomers Using Computational Spectroscopy. <i>Australian Journal of Chemistry</i> , 2020, 73, 813.	0.5	1

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37	Pyrene-alt-dibenzothiophene-S,S-dioxide copolymers for highly efficient photocatalytic hydrogen production: The role of linking pattern. <i>Applied Surface Science</i> , 2019, 495, 143537.	3.1	27
38	Switching on optical properties of D- $\pi$ -A DSSC sensitizers from $\pi$ -spacers towards machine learning. <i>Solar Energy</i> , 2019, 188, 1189-1200.	2.9	21
39	First-principle investigation of hydrogen solubility and diffusivity in transition metal-doped vanadium membranes and their mechanical properties. <i>Journal of Alloys and Compounds</i> , 2019, 805, 747-756.	2.8	28
40	Structural and Spectroscopic Study of the Tyrosine Kinase Inhibitor PD-153035. <i>Biophysical Journal</i> , 2019, 116, 568a.	0.2	0
41	Synergetic Effect of Perfluorooctanoic Acid on the Preparation of Poly(3,4-ethylenedioxythiophene): Lignosulfonate Aqueous Dispersions with High Film Conductivity. <i>ChemistrySelect</i> , 2019, 4, 11406-11412.	0.7	7
42	Enhanced photocatalytic activity of g-C <sub>3</sub> N <sub>4</sub> /MnO composites for hydrogen evolution under visible light. <i>Dalton Transactions</i> , 2019, 48, 14864-14872.	1.6	16
43	Rational use of ligand to shift the UV-vis spectrum of Ru-complex sensitizer dyes for DSSC applications. <i>Radiation Physics and Chemistry</i> , 2019, 161, 66-71.	1.4	10
44	Element-free Galerkin scaled boundary method based on moving Kriging interpolation for steady heat conduction analysis. <i>Engineering Analysis With Boundary Elements</i> , 2019, 106, 440-451.	2.0	15
45	Effects of Mo alloying on stability and diffusion of hydrogen in the Nb <sub>16</sub> H phase: a first-principles investigation. <i>RSC Advances</i> , 2019, 9, 19495-19500.	1.7	5
46	Radiation Damage Mechanisms of Chemotherapeutically Active Nitroimidazole Derived Compounds. <i>Frontiers in Chemistry</i> , 2019, 7, 329.	1.8	10
47	Facile preparation of MnO/nitrogen-doped porous carbon nanotubes composites and their application in energy storage. <i>Journal of Power Sources</i> , 2019, 426, 33-39.	4.0	28
48	Methodologies in Spectral Tuning of DSSC Chromophores through Rational Design and Chemical-Structure Engineering. <i>Materials</i> , 2019, 12, 4024.	1.3	5
49	Conjugated Microporous Polymers with Tunable Electronic Structure for High-Performance Potassium-Ion Batteries. <i>ACS Nano</i> , 2019, 13, 745-754.	7.3	162
50	Significant improved selectivity of a fluorescent sensor for Al <sup>3+</sup> made from a fluorinated rhodamine B Schiff base. <i>Research on Chemical Intermediates</i> , 2019, 45, 1815-1827.	1.3	4
51	Building an electron push-pull system of linear conjugated polymers for improving photocatalytic hydrogen evolution efficiency. <i>Polymer Bulletin</i> , 2019, 76, 3195-3206.	1.7	20
52	Resveratrol's Hidden Hand: A Route to the Optical Detection of Biomolecular Binding. <i>Journal of Physical Chemistry B</i> , 2018, 122, 2841-2850.	1.2	3
53	Conformational Plasticity in Tyrosine Kinase Inhibitor-Kinase Interactions Revealed with Fluorescence Spectroscopy and Theoretical Calculations. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4667-4679.	1.2	7
54	Conjugated Microporous Polytetra(2-thienyl)ethylene as High Performance Anode Material for Lithium- and Sodium-Ion Batteries. <i>Macromolecular Chemistry and Physics</i> , 2018, 219, 1700524.	1.1	39

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55	Rational design of donor-acceptor conjugated microporous polymers for photocatalytic hydrogen production. <i>Applied Catalysis B: Environmental</i> , 2018, 228, 1-9.	10.8	215
56	Hypercrosslinked silole-containing microporous organic polymers with N-functionalized pore surfaces for gas storage and separation. <i>Journal of Applied Polymer Science</i> , 2018, 135, 45907.	1.3	12
57	Hierarchical porous carbon activated by CaCO <sub>3</sub> from pigskin collagen for CO <sub>2</sub> and H <sub>2</sub> adsorption. <i>Microporous and Mesoporous Materials</i> , 2018, 260, 172-179.	2.2	36
58	Effect of Linking Pattern of Dibenzothiophene-S,S-dioxide-Containing Conjugated Microporous Polymers on the Photocatalytic Performance. <i>Macromolecules</i> , 2018, 51, 9502-9508.	2.2	113
59	Electronic structure and intramolecular interactions in three methoxyphenol isomers. <i>Journal of Chemical Physics</i> , 2018, 149, 134312.	1.2	13
60	A novel off-on fluorescent chemosensor for Al <sup>3+</sup> derived from a 4,5-diazafluorene Schiff base derivative. <i>RSC Advances</i> , 2018, 8, 31889-31894.	1.7	21
61	Quantum chemical approach for positron annihilation spectra of atoms and molecules beyond plane-wave approximation. <i>Journal of Chemical Physics</i> , 2018, 148, 184110.	1.2	6
62	The effect of molecular structure and fluorination on the properties of pyrene-benzothiadiazole-based conjugated polymers for visible-light-driven hydrogen evolution. <i>Polymer Chemistry</i> , 2018, 9, 4468-4475.	1.9	56
63	Dibenzothiophene Dioxide Based Conjugated Microporous Polymers for Visible-Light-Driven Hydrogen Production. <i>ACS Catalysis</i> , 2018, 8, 8590-8596.	5.5	202
64	Synthesis and Photovoltaic Properties of 2D-Conjugated Polymers Based on Alkylthiothienyl-Substituted Benzodithiophene and Different Accepting Units. <i>Polymers</i> , 2018, 10, 331.	2.0	11
65	A heptacyclic carbon-oxygen-bridged ladder-type building block for D-A acceptors. <i>Materials Chemistry Frontiers</i> , 2018, 2, 1716-1719.	3.2	34
66	Insights into the dissociative ionization of glycine by PEPICO experiments. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22841-22848.	1.3	13
67	Toward High Performance Thiophene-Containing Conjugated Microporous Polymer Anodes for Lithium-Ion Batteries through Structure Design. <i>Advanced Functional Materials</i> , 2018, 28, 1705432.	7.8	162
68	Reduced order model analysis method via proper orthogonal decomposition for nonlinear transient heat conduction problems. <i>Scientia Sinica: Physica, Mechanica Et Astronomica</i> , 2018, 48, 124603.	0.2	3
69	Dominant Carbons in trans- and cis-Resveratrol Isomerization. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4745-4755.	1.2	36
70	Perylene-Containing Conjugated Microporous Polymers for Photocatalytic Hydrogen Evolution. <i>Macromolecular Chemistry and Physics</i> , 2017, 218, 1700049.	1.1	71
71	Low-bandgap conjugated polymers based on alkylthiothienyl-substituted benzodithiophene for efficient bulk heterojunction polymer solar cells. <i>Polymer</i> , 2017, 122, 96-104.	1.8	18
72	Control Synthesis of Tubular Hyper-Cross-Linked Polymers for Highly Porous Carbon Nanotubes. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 20779-20786.	4.0	77

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73	Porous carbons derived from hypercrosslinked porous polymers for gas adsorption and energy storage. <i>Carbon</i> , 2017, 114, 608-618.	5.4	170
74	Synthesis and Characterization of Functional Triphenylphosphine-Containing Microporous Organic Polymers for Gas Storage and Separation. <i>Macromolecular Chemistry and Physics</i> , 2017, 218, 1700275.	1.1	8
75	Exploring the optical reporting characteristics of drugs: UV-Vis spectra and conformations of the tyrosine kinase inhibitor SKF86002. <i>New Journal of Chemistry</i> , 2017, 41, 14567-14573.	1.4	4
76	Tetra-armed conjugated microporous polymers for gas adsorption and photocatalytic hydrogen evolution. <i>Science China Chemistry</i> , 2017, 60, 1075-1083.	4.2	46
77	Micro-solvation of tyrosine-kinase inhibitor AG1478 explored with fluorescence spectroscopy and computational chemistry. <i>RSC Advances</i> , 2017, 7, 31725-31735.	1.7	5
78	Solvatochromism and linear solvation energy relationship of the kinase inhibitor SKF86002. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 170, 226-233.	2.0	4
79	A pH-induced conformational switch in a tyrosine kinase inhibitor identified by electronic spectroscopy and quantum chemical calculations. <i>Scientific Reports</i> , 2017, 7, 16271.	1.6	3
80	Synthesis and Gas Sorption Properties of Microporous Poly(arylene ethynylene) Frameworks. <i>Acta Chimica Sinica</i> , 2017, 75, 473.	0.5	4
81	Application Of Computational Methods To The Rational Design Of Photoactive Materials For Solar Cells. , 2017, , 179-207.		0
82	Conformation Analysis of Ferrocene and Decamethylferrocene via Full-Potential Modeling of XANES and XAFS Spectra. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2792-2796.	2.1	13
83	Combined SRCT & FXCT – The next steps. <i>Journal of Instrumentation</i> , 2016, 11, C03048-C03048.	0.5	3
84	Microporous organic polymers based on tetraethynyl building blocks with N-functionalized pore surfaces: synthesis, porosity and carbon dioxide sorption. <i>RSC Advances</i> , 2016, 6, 113826-113833.	1.7	15
85	UV-Vis spectroscopy and solvatochromism of the tyrosine kinase inhibitor AG-1478. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 164, 128-132.	2.0	14
86	Accurate X-ray Absorption Spectra of Dilute Systems: Absolute Measurements and Structural Analysis of Ferrocene and Decamethylferrocene. <i>Journal of Physical Chemistry C</i> , 2016, 120, 9399-9418.	1.5	20
87	Reinterpretation of Dynamic Vibrational Spectroscopy to Determine the Molecular Structure and Dynamics of Ferrocene. <i>Chemistry - A European Journal</i> , 2016, 22, 18019-18026.	1.7	13
88	Two conformers of a tyrosine kinase inhibitor (AG-1478) disclosed using simulated UV-Vis absorption spectroscopy. <i>New Journal of Chemistry</i> , 2016, 40, 8296-8304.	1.4	16
89	X-ray Photoemission Spectra and Electronic Structure of Coumarin and its Derivatives. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7080-7087.	1.1	6
90	How different is pyrimidine as a core component of DNA base from its diazine isomers: A DFT study?. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1836-1845.	1.0	5

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91	Synthesis and photovoltaic properties of donor-acceptor conjugated polymers based on 4,7-dithienyl-2,1,3-benzothiadiazole functionalized silole. <i>Synthetic Metals</i> , 2016, 220, 433-439.	2.1	15
92	A Turn-on and Reversible Fluorescence Sensor for Zinc Ion Based on 4,5-Diazafluorene Schiff Base. <i>Journal of Fluorescence</i> , 2016, 26, 1555-1561.	1.3	19
93	Molecular dynamics studies on the buffalo prion protein. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 762-777.	2.0	7
94	Shifting UV-vis absorption spectrum through rational structural modifications of zinc porphyrin photoactive compounds. <i>RSC Advances</i> , 2016, 6, 15345-15353.	1.7	17
95	How similar is the electronic structures of $\beta$ -lactam and alanine?. <i>Radiation Physics and Chemistry</i> , 2016, 119, 1-8.	1.4	5
96	Novel 4,5-diazafluorene-based Schiff base derivatives as Al <sup>3+</sup> ions fluorescence turn-on sensors. <i>Synthetic Metals</i> , 2016, 217, 37-42.	2.1	12
97	A review on the salt bridge ASP177-ARG163 (O <sup>-</sup> N) of wild-type rabbit prion protein. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 1020-1028.	2.0	6
98	Discovery of Novel Peptidomimetics as Irreversible CHIKV NsP <sup>2</sup> Protease Inhibitors Using Quantum Mechanical-Based Ligand Descriptors. <i>Chemical Biology and Drug Design</i> , 2015, 86, 1518-1527.	1.5	18
99	Ferrocene Orientation Determined Intramolecular Interactions Using Energy Decomposition Analysis. <i>Materials</i> , 2015, 8, 7723-7737.	1.3	13
100	Photoelectron Spectra and Electronic Structures of the Radiosensitizer Nimorazole and Related Compounds. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9986-9995.	1.1	19
101	Theoretical study of valence orbital response to guanine tautomerization in coordinate and momentum spaces. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2015, 48, 205101.	0.6	3
102	Sitting above the maze: recent model discoveries in molecular science. <i>Molecular Simulation</i> , 2015, 41, 205-229.	0.9	4
103	Targeting the Achilles heel of the hepatitis B virus: a review of current treatments against covalently closed circular DNA. <i>Drug Discovery Today</i> , 2015, 20, 548-561.	3.2	22
104	The d-electrons of Fe in ferrocene: the excess orbital energy spectrum (EOES). <i>RSC Advances</i> , 2015, 5, 11933-11941.	1.7	16
105	Molecular dynamics studies on the NMR structures of rabbit prion protein wild type and mutants: surface electrostatic charge distributions. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 1326-1335.	2.0	12
106	Enhanced solubilization of large-diameter single-walled carbon nanotubes with amino-functionalized dipylene nanotweezers. <i>Journal of Materials Science</i> , 2015, 50, 6032-6040.	1.7	9
107	Electronic structures of hexane isomers studied using quantum mechanics and graph theory. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550014.	1.8	5
108	Synthesis of $\pi$ -Extended Dithienobenzodithiophene-Containing Medium Bandgap Copolymers and Their Photovoltaic Application. <i>Journal of Macromolecular Science - Pure and Applied Chemistry</i> , 2015, 52, 934-941.	1.2	11

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109	Synthesis and characterization of alternating and random conjugated polymers derived from dithieno[2,3-d:2â€²,3â€²-dâ€²]benzo[1,2-b:4,5-bâ€²]dithiophene and 2,1,3-benzothiadiazole derivatives. <i>Polymer</i> 1.3 Journal, 2015, 47, 803-809.		8
110	Throughput based temporal verification for monitoring large batch of parallel processes. , 2014, , .		15
111	Graphene oxide nanoparticles for enhanced photothermal cancer cell therapy under the irradiation of a femtosecond laser beam. <i>Journal of Biomedical Materials Research - Part A</i> , 2014, 102, 2181-2188.	2.1	54
112	A New Particle Swarm Optimization-Based Strategy for Cost-Effective Data Placement in Scientific Cloud Workflows. <i>Lecture Notes in Electrical Engineering</i> , 2014, , 115-120.	0.3	4
113	From building blocks of proteins to drugs: a quantum chemical study on structureâ€“property relationships of phenylalanine, tyrosine and dopa. <i>RSC Advances</i> , 2014, 4, 8617.	1.7	9
114	Differentiation of alkane isomers through binding energy spectra and total momentum cross sections. <i>New Journal of Chemistry</i> , 2014, 38, 1031.	1.4	12
115	Valence orbital response to methylation of uracil. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 314-320.	1.0	0
116	Fine Tuning of Fluorene-Based Dye Structures for High-Efficiency <i>p</i> -Type Dye-Sensitized Solar Cells. <i>ACS Applied Materials &amp; Interfaces</i> , 2014, 6, 10614-10622.	4.0	64
117	Hypercrosslinked microporous organic polymer networks derived from silole-containing building blocks. <i>Polymer</i> , 2014, 55, 5746-5750.	1.8	36
118	First-principles study of Carbz-PAHTDDT dye sensitizer and two Carbz-derived dyes for dye sensitized solar cells. <i>Journal of Molecular Modeling</i> , 2014, 20, 2177.	0.8	17
119	Modulated Charge Injection in <i>p</i> -Type Dye-Sensitized Solar Cells Using Fluorene-Based Light Absorbers. <i>ACS Applied Materials &amp; Interfaces</i> , 2014, 6, 3448-3454.	4.0	48
120	Logistics scheduling based on cloud business workflows. , 2014, , .		3
121	Calculations of gamma-ray spectral profiles of linear alkanes in the positron annihilation process. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2014, 196, 146-151.	0.8	8
122	Structures of Cycloserine and 2-Oxazolidinone Probed by X-ray Photoelectron Spectroscopy: Theory and Experiment. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3645-3654.	1.1	8
123	Discovery of new HER2/EGFR dual kinase inhibitors based on the anilinoquinazoline scaffold as potential anti-cancer agents. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2014, 29, 215-222.	2.5	27
124	A Survey and a Molecular Dynamics Study on the (Central) Hydrophobic Region of Prion Proteins. <i>Current Pharmaceutical Biotechnology</i> , 2014, 15, 1026-1048.	0.9	1
125	Fragment based electronic structural analysis of <i>l</i> -phenylalanine using calculated ionization spectroscopy and dual space analysis. <i>RSC Advances</i> , 2014, 4, 60597-60608.	1.7	4
126	In silico design: Extended molecular dynamic simulations of a new series of dually acting inhibitors against EGFR and HER2. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 44, 220-231.	1.3	26



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127	Theoretical investigation of the electron capture and loss processes in the collisions of He <sup>2+</sup> + Ne. Journal of Chemical Physics, 2013, 139, 084321.	1.2	7
128	A study of aliphatic amino acids using simulated vibrational circular dichroism and Raman optical activity spectra. European Physical Journal D, 2013, 67, 1.	0.6	21
129	A facile approach to synthesize SiO <sub>2</sub> @Re <sub>2</sub> O <sub>3</sub> (Re=Y, Eu, La, Sm, Tb, Pr) hollow sphere and its application in drug release. Nanoscale Research Letters, 2013, 8, 435.	3.1	3
130	Density functional study of Cu <sup>2+</sup> -phenylalanine complex under micro-solvation environment. Journal of Molecular Graphics and Modelling, 2013, 45, 180-191.	1.3	10
131	Adsorption of Cytosine and AZA Derivatives of Cytidine on Au Single Crystal Surfaces. Journal of Physical Chemistry C, 2013, 117, 18423-18433.	1.5	18
132	Study of Nano-Hydroxyapatite Adsorption in Heavy Metals. Advanced Materials Research, 2013, 777, 15-18.	0.3	3
133	Toward rational design of organic dye sensitized solar cells (DSSCs): An application to the TA-St-CA dye. Journal of Molecular Graphics and Modelling, 2013, 40, 64-71.	1.3	42
134	Docking Positrophilic Electrons into Molecular Attractive Potentials of Fluorinated Methanes. Journal of the Physical Society of Japan, 2013, 82, 104301.	0.7	11
135	The impact of candidate display styles for Japanese and Chinese characters on input efficiency. International Journal of Human Computer Studies, 2013, 71, 236-249.	3.7	2
136	Gamma-ray spectra of methane in the positron-electron annihilation process. Radiation Physics and Chemistry, 2013, 85, 59-63.	1.4	16
137	Simultaneous Discrimination of Diameter, Handedness, and Metallicity of Single-Walled Carbon Nanotubes with Chiral Diporphyrin Nanocalipers. Journal of the American Chemical Society, 2013, 135, 4805-4814.	6.6	45
138	Assessment of new anti-HER2 ligands using combined docking, QM/MM scoring and MD simulation. Journal of Molecular Graphics and Modelling, 2013, 40, 91-98.	1.3	18
139	Inheritance and correlation of nucleic acid pyrimidine bases. International Journal of Quantum Chemistry, 2013, , n/a-n/a.	1.0	0
140	Gamma-ray spectra of hexane (C <sub>6</sub> H <sub>14</sub> ) in positron-electron annihilation process. Radiation Physics and Chemistry, 2013, 89, 14-19.	1.4	17
141	Enrichment of Large-Diameter Single-Walled Carbon Nanotubes (SWNTs) with Metallo-Octaethylporphyrins. Materials, 2013, 6, 3064-3078.	1.3	9
142	Inheritance and correlation of nucleic acid pyrimidine bases. International Journal of Quantum Chemistry, 2013, , n/a-n/a.	1.0	1
143	DFT Study on the Conformational and Vibrational Properties of 3'-Deoxycytidine and Its Analogues. International Journal of Chemistry, 2013, 5, .	0.3	0
144	In Silico Investigation of Lactone and Thiolactone Inhibitors in Bacterial Quorum Sensing Using Molecular Modeling. International Journal of Chemistry, 2013, 5, .	0.3	13

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