Feng Wang

List of Publications by Year
in descending order

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	Carbon Nanotubes with Titanium Nitride as a Lowâ€Cost Counterâ€Electrode Material for Dyeâ€Sensitized Solar Cells. Angewandte Chemie - International Edition, 2010, 49, 3653-3656.	7.2	554
2	Rational design of donor-Ï€-acceptor conjugated microporous polymers for photocatalytic hydrogen production. Applied Catalysis B: Environmental, 2018, 228, 1-9.	10.8	215
3	Dibenzothiophene Dioxide Based Conjugated Microporous Polymers for Visible-Light-Driven Hydrogen Production. ACS Catalysis, 2018, 8, 8590-8596.	5.5	202
4	Porous carbons derived from hypercrosslinked porous polymers for gas adsorption and energy storage. Carbon, 2017, 114, 608-618.	5.4	170
5	Conjugated Microporous Polymers with Tunable Electronic Structure for High-Performance Potassium-Ion Batteries. ACS Nano, 2019, 13, 745-754.	7.3	162
6	Toward High Performance Thiopheneâ€Containing Conjugated Microporous Polymer Anodes for Lithiumâ€Ion Batteries through Structure Design. Advanced Functional Materials, 2018, 28, 1705432.	7.8	162
7	Conjugated Fluorene and Silole Copolymers:â€‰ Synthesis, Characterization, Electronic Transition, Light Emission, Photovoltaic Cell, and Field Effect Hole Mobility. Macromolecules, 2005, 38, 2253-2260.	2.2	161
8	Boosting the Photocatalytic Hydrogen Evolution Activity for Dâ€“Ï€â€“A Conjugated Microporous Polymers by Statistical Copolymerization. Advanced Materials, 2021, 33, e2008498.	11.1	143
9	Adenine Tautomers:â€‰ Relative Stabilities, Ionization Energies, and Mismatch with Cytosine. Journal of Physical Chemistry A, 2006, 110, 4012-4020.	1.1	115
10	Effect of Linking Pattern of Dibenzothiophene-S,S-dioxide-Containing Conjugated Microporous Polymers on the Photocatalytic Performance. Macromolecules, 2018, 51, 9502-9508.	2.2	113
11	A Comprehensive Review on Separation Methods and Techniques for Single-Walled Carbon Nanotubes. Materials, 2010, 3, 3818-3844.	1.3	91
12	Substituent effect of conjugated microporous polymers on the photocatalytic hydrogen evolution activity. Journal of Materials Chemistry A, 2020, 8, 2404-2411.	5.2	91
13	Differentiation of ferrocene D5d and D5h conformers using IR spectroscopy. Journal of Organometallic Chemistry, 2012, 713, 51-59.	0.8	90
14	Simultaneous Discrimination of Handedness and Diameter of Single-Walled Carbon Nanotubes (SWNTs) with Chiral Diporphyrin Nanotweezers Leading to Enrichment of a Single Enantiomer of (6,5)-SWNTs. Journal of the American Chemical Society, 2010, 132, 10876-10881.	6.6	88
15	Theoretical Investigation of Single and Double Transition Metals Anchored on Graphyne Monolayer for Nitrogen Reduction Reaction. Journal of Physical Chemistry C, 2020, 124, 15295-15301.	1.5	79
16	Control Synthesis of Tubular Hyper-Cross-Linked Polymers for Highly Porous Carbon Nanotubes. ACS Applied Materials & Interfaces, 2017, 9, 20779-20786.	4.0	77
17	Realizing high hydrogen evolution activity under visible light using narrow band gap organic photocatalysts. Chemical Science, 2021, 12, 1796-1802.	3.7	77
18	Differential attraction and repulsion of Staphylococcus aureus and Pseudomonas aeruginosa on molecularly smooth titanium films. Scientific Reports, 2011, 1, 165.	1.6	76

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19	Peryleneâ€Containing Conjugated Microporous Polymers for Photocatalytic Hydrogen Evolution. Macromolecular Chemistry and Physics, 2017, 218, 1700049.	1.1	71
20	Understanding glycine conformation through molecular orbitals. Journal of Chemical Physics, 2005, 123, 214307.	1.2	64
21	New Diagnostic of the Most Populated Conformer of Tetrahydrofuran in the Gas Phase. Journal of Physical Chemistry A, 2007, 111, 4927-4933.	1.1	64
22	Fine Tuning of Fluorene-Based Dye Structures for High-Efficiency p-Type Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2014, 6, 10614-10622.	4.0	64
23	Plasma-Enhanced Synthesis of Bioactive Polymeric Coatings from Monoterpene Alcohols: A Combined Experimental and Theoretical Study. Biomacromolecules, 2010, 11, 2016-2026.	2.6	63
24	Silver nanoparticleâ€“carbon nanotube hybrid films: Preparation and electrochemical sensing. Electrochimica Acta, 2012, 74, 111-116.	2.6	63
25	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
26	Assessment of Quantum Mechanical Models Based on Resolved Orbital Momentum Distributions of n-Butane in the Outer Valence Shell. Journal of Physical Chemistry A, 2003, 107, 10199-10207.	1.1	60
27	Experimental and Theoretical Electron Momentum Spectroscopic Study of the Valence Electronic Structure of Tetrahydrofuran under Pseudorotation. Journal of Physical Chemistry A, 2008, 112, 11078-11087.	1.1	56
28	The effect of molecular structure and fluorination on the properties of pyrene-benzothiadiazole-based conjugated polymers for visible-light-driven hydrogen evolution. Polymer Chemistry, 2018, 9, 4468-4475.	1.9	56
29	Graphene oxide nanoparticles for enhanced photothermal cancer cell therapy under the irradiation of a femtosecond laser beam. Journal of Biomedical Materials Research - Part A, 2014, 102, 2181-2188.	2.1	54
30	Conjugated random and alternating 2,3,4,5-tetraphenylsilole-containing polyfluorenes: Synthesis, characterization, strong solution photoluminescence, and light-emitting diodes. Polymer, 2005, 46, 8422-8429.	1.8	53
31	Modulated Charge Injection in p-Type Dye-Sensitized Solar Cells Using Fluorene-Based Light Absorbers. ACS Applied Materials & Interfaces, 2014, 6, 3448-3454.	4.0	48
32	Tetra-armed conjugated microporous polymers for gas adsorption and photocatalytic hydrogen evolution. Science China Chemistry, 2017, 60, 1075-1083.	4.2	46
33	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
34	Norbornane: An investigation into its valence electronic structure using electron momentum spectroscopy, and density functional and Greenâ€™s function theories. Journal of Chemical Physics, 2004, 121, 10525-10541.	1.2	43
35	ADENINE TAUTOMER ELECTRONIC STRUCTURAL SIGNATURES STUDIED USING DUAL SPACE ANALYSIS. Journal of Theoretical and Computational Chemistry, 2005, 04, 247-264.	1.8	43
36	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

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37	Poly(dibenzothiophene-S,S-dioxide) with visible light-induced hydrogen evolution rate up to 44.2â€¯mmol hâ¯1 gâ¯1 promoted by K2HPO4. Applied Catalysis B: Environmental, 2020, 261, 118230.	10.8	40
38	Dibenzothiophene-S,S-dioxide-containing conjugated polymer with hydrogen evolution rate up to 147ÂmmolÂgâ¯1 hâ¯1. Applied Catalysis B: Environmental, 2022, 307, 121144.	10.8	40
39	Diameter-based separation of single-walled carbon nanotubes through selective extraction with dipyrene nanotweezers. Chemical Science, 2011, 2, 862.	3.7	39
40	Conjugated Microporous Polytetra(2â€Thienyl)ethylene as High Performance Anode Material for Lithiumâ€•and Sodiumâ€•Ion Batteries. Macromolecular Chemistry and Physics, 2018, 219, 1700524.	1.1	39
41	Coexistence of 1,3-butadiene conformers in ionization energies and Dyson orbitals. Journal of Chemical Physics, 2005, 123, 124315.	1.2	38
42	Electronic Structure of the Azide Group in 3Â¢-Azido-3Â¢-deoxythymidine (AZT) Compared to Small Azide Compounds. Molecules, 2009, 14, 2656-2668.	1.7	37
43	Orbital Signatures of Methyl inl-Alanine. Journal of Physical Chemistry B, 2006, 110, 9713-9719.	1.2	36
44	Hypercrosslinked microporous organic polymer networks derived from silole-containing building blocks. Polymer, 2014, 55, 5746-5750.	1.8	36
45	Dominant Carbons in trans- and cis-Resveratrol Isomerization. Journal of Physical Chemistry B, 2017, 121, 4745-4755.	1.2	36
46	Hierarchical porous carbon activated by CaCO3 from pigskin collagen for CO2 and H2 adsorption. Microporous and Mesoporous Materials, 2018, 260, 172-179.	2.2	36
47	Microwave spectra of the Neâ€“N2 Van der Waals complex: Experiment and theory. Journal of Chemical Physics, 1998, 109, 5420-5432.	1.2	34
48	A Density Functional Theory and Electron Momentum Spectroscopy Study into the Complete Valence Electronic Structure of Cubane. Journal of the American Chemical Society, 2000, 122, 3892-3900.	6.6	34
49	A heptacyclic carbonâ€“oxygen-bridged ladder-type building block for Aâ€“Dâ€“A acceptors. Materials Chemistry Frontiers, 2018, 2, 1716-1719.	3.2	34
50	Electronic Structure Study of the N2O Isomers Using Post-Hartreeâ¯Fock and Density Functional Theory Calculations. Journal of Physical Chemistry A, 2000, 104, 1304-1310.	1.1	33
51	Methylation of Zebularine: A Quantum Mechanical Study Incorporating Interactive 3D pdf Graphs. Journal of Physical Chemistry B, 2009, 113, 11496-11504.	1.2	33
52	Optical Resolution of Single-Walled Carbon Nanotubes through Molecular Recognition with Chiral Diporphyrin Nanotweezers. Chemistry Letters, 2010, 39, 1022-1027.	0.7	30
53	Dynamical (e,2e) studies of tetrahydrofurfuryl alcohol. Journal of Chemical Physics, 2012, 136, 244301.	1.2	30
54	Structure evolution of azo-fused conjugated microporous polymers for high performance lithium-ion batteries anodes. Journal of Power Sources, 2020, 453, 227868.	4.0	30

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55	Investigation into the Valence Electronic Structure of Norbornene Using Electron Momentum Spectroscopy, Green's Function, and Density Functional Theories. Journal of Physical Chemistry A, 2005, 109, 9324-9340.	1.1	28
56	Correlation of electronic structures of three cyclic dipeptides with their photoemission spectra. Journal of Chemical Physics, 2010, 133, 174319.	1.2	28
57	First-principle investigation of hydrogen solubility and diffusivity in transition metal-doped vanadium membranes and their mechanical properties. Journal of Alloys and Compounds, 2019, 805, 747-756.	2.8	28
58	Facile preparation of MnO/nitrogen-doped porous carbon nanotubes composites and their application in energy storage. Journal of Power Sources, 2019, 426, 33-39.	4.0	28
59	Improved selectivity in discriminating handedness and diameter of single-walled carbon nanotubes with N-substituted 3,6-carbazolylene-bridged chiral diporphyrin nanotweezers. Nanoscale, 2011, 3, 4117.	2.8	27
60	Photoelectron spectra and structures of three cyclic dipeptides: PhePhe, TyrPro, and HisGly. Journal of Chemical Physics, 2012, 136, 124301.	1.2	27
61	Stereochemical analysis of ferrocene and the uncertainty of fluorescence XAFS data. Journal of Synchrotron Radiation, 2012, 19, 145-158.	1.0	27
62	Discovery of new HER2/EGFR dual kinase inhibitors based on the anilinoquinazoline scaffold as potential anti-cancer agents. Journal of Enzyme Inhibition and Medicinal Chemistry, 2014, 29, 215-222.	2.5	27
63	Pyrene-alt-dibenzothiophene-S,S-dioxide copolymers for highly efficient photocatalytic hydrogen production: The role of linking pattern. Applied Surface Science, 2019, 495, 143537.	3.1	27
64	Orbital based electronic structural signatures of the guanine keto G-7H/G-9H tautomer pair as studied using dual space analysis. Biophysical Chemistry, 2006, 121, 105-120.	1.5	26
65	Inner-shell chemical shift of DNA/RNA bases and inheritance from their parent purine and pyrimidine. Journal of Synchrotron Radiation, 2008, 15, 624-631.	1.0	26
66	Valence orbital response to pseudorotation of tetrahydrofuran: A snapshot using dual space analysis. Journal of Chemical Physics, 2008, 128, 125102.	1.2	26
67	In silico design: Extended molecular dynamic simulations of a new series of dually acting inhibitors against EGFR and HER2. Journal of Molecular Graphics and Modelling, 2013, 44, 220-231.	1.3	26
68	Theoretical investigation of molybdenum/tungsten-vanadium solid solution alloy membranes: Thermodynamic stability and hydrogen permeation. Journal of Membrane Science, 2020, 608, 118200.	4.1	26
69	The attachment of amino fragment to purine: inner-shell structures and spectra. Journal of Synchrotron Radiation, 2008, 15, 151-157.	1.0	25
70	Optical Resolution and Diameter-Based Enrichment of Single-Walled Carbon Nanotubes through Simultaneous Recognition of Their Helicity and Diameter with Chiral Monoporphyrin. Journal of Physical Chemistry C, 2009, 113, 9108-9113.	1.5	25
71	Intramolecular interactions of L-phenylalanine revealed by inner shell chemical shift. Journal of Chemical Physics, 2009, 131, 044321.	1.2	24
72	A high performance and low cost poly(dibenzothiophene-S,S-dioxide)@TiO₂ composite with hydrogen evolution rate up to 51.5 mmol h^{â˜'1} g^{â˜'1}. Journal of Materials Chemistry A, 2020, 8, 18292-18301.	5.2	23

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73	Valence bond and molecular orbital studies of three N2O isomers, and valence bond representations for some azide decompositions. Journal of Molecular Modeling, 2001, 7, 271-277.	0.8	22
74	Preferential extraction of left- or right-handed single-walled carbon nanotubes by use of chiral diporphyrin nanotweezers. Organic and Biomolecular Chemistry, 2012, 10, 5830.	1.5	22
75	Targeting the Achilles heel of the hepatitis B virus: a review of current treatments against covalently closed circular DNA. Drug Discovery Today, 2015, 20, 548-561.	3.2	22
76	Ab initio rotationally resolved infrared spectrum of potassium-lithium (K2Li+). The Journal of Physical Chemistry, 1992, 96, 6158-6165.	2.9	21
77	Inner valence shell bonding mechanism of n-butane studied using orbital momentum distributions of its conformational isomers. Journal of Physics B: Atomic, Molecular and Optical Physics, 2004, 37, 557-569.	0.6	21
78	Effect of positronâ€“atom interactions on the annihilation gamma spectra of molecules. New Journal of Physics, 2012, 14, 035021.	1.2	21
79	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
80	A novel off-on fluorescent chemosensor for Al³⁺derived from a 4,5-diazafluorene Schiff base derivative. RSC Advances, 2018, 8, 31889-31894.	1.7	21
81	Switching on optical properties of D-Ï€-A DSSC sensitizers from Ï€-spacers towards machine learning. Solar Energy, 2019, 188, 1189-1200.	2.9	21
82	Accurate X-ray Absorption Spectra of Dilute Systems: Absolute Measurements and Structural Analysis of Ferrocene and Decamethylferrocene. Journal of Physical Chemistry C, 2016, 120, 9399-9418.	1.5	20
83	Building an electron pushâ€“pull system of linear conjugated polymers for improving photocatalytic hydrogen evolution efficiency. Polymer Bulletin, 2019, 76, 3195-3206.	1.7	20
84	Bisulfoneâ€Functionalized Organic Polymer Photocatalysts for Highâ€Performance Hydrogen Evolution. ChemSusChem, 2020, 13, 369-375.	3.6	20
85	The electronic structural information from core orbitals of norbornadiene, norbornene and norbornane. Computational and Theoretical Chemistry, 2005, 728, 31-42.	1.5	19
86	Intramolecular interactions of <scp>L</scp>â€phenylalanine: Valence ionization spectra and orbital momentum distributions of its fragment molecules. Journal of Computational Chemistry, 2011, 32, 525-535.	1.5	19
87	Photoelectron Spectra and Electronic Structures of the Radiosensitizer Nimorazole and Related Compounds. Journal of Physical Chemistry A, 2015, 119, 9986-9995.	1.1	19
88	A Turn-on and Reversible Fluorescence Sensor for Zinc Ion Based on 4,5-Diazafluorene Schiff Base. Journal of Fluorescence, 2016, 26, 1555-1561.	1.3	19
89	An electron momentum spectroscopy and density functional theory study of the outer valence electronic structure of stella-2,6-dione. Journal of Physics B: Atomic, Molecular and Optical Physics, 2003, 36, 3155-3171.	0.6	18
90	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

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91	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
92	Discovery of Novel Peptidomimetics as Irreversible <scp>CHIKV</scp> Ns<scp>P</scp>2 Protease Inhibitors Using Quantum Mechanicalâ€Based Ligand Descriptors. Chemical Biology and Drug Design, 2015, 86, 1518-1527.	1.5	18
93	Low-bandgap conjugated polymers based on alkylthiothienyl-substituted benzodithiophene for efficient bulk heterojunction polymer solar cells. Polymer, 2017, 122, 96-104.	1.8	18
94	Thiophene-rich conjugated microporous polymers as anode materials for high performance lithium- and sodium-ion batteries. Solid State Ionics, 2020, 347, 115247.	1.3	18
95	Dipole moment surfaces and the mid- and far-IR spectra of N2-Ar. Journal of Chemical Physics, 2000, 113, 98-106.	1.2	17
96	Comprehensive Experimental and Theoretical Study into the Complete Valence Electronic Structure of Norbornadiene. Journal of Physical Chemistry A, 2002, 106, 9573-9581.	1.1	17
97	Definitive confirmation for through-space bond dominance in the outermost Ï€-orbitals of norbornadiene. Journal of Electron Spectroscopy and Related Phenomena, 2002, 123, 389-395.	0.8	17
98	Blue shifted intramolecular Câ^'HÂ·Â·Â·O improper hydrogen bonds in conformers of zidovudine. Chemical Physics Letters, 2010, 493, 358-363.	1.2	17
99	Positron scattering from chiral enantiomers. Physical Review A, 2012, 85, .	1.0	17
100	Gamma-ray spectra of hexane (C6H14) in positronâ€“electron annihilation process. Radiation Physics and Chemistry, 2013, 89, 14-19.	1.4	17
101	First-principles study of Carbz-PAHTDDT dye sensitizer and two Carbz-derived dyes for dye sensitized solar cells. Journal of Molecular Modeling, 2014, 20, 2177.	0.8	17
102	Shifting UV-vis absorption spectrum through rational structural modifications of zinc porphyrin photoactive compounds. RSC Advances, 2016, 6, 15345-15353.	1.7	17
103	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
104	Exploring the electronic structure of 2,6-stelladione from momentum space I: the p-dominant molecular orbitals in the outer valence shell. Chemical Physics Letters, 2003, 382, 217-225.	1.2	16
105	Interfacial stress transfer of fiber pullout for carbon nanotubes with a composite coating. Journal of Materials Science, 2007, 42, 4191-4196.	1.7	16
106	Gamma-ray spectra of methane in the positronâ€“electron annihilationprocess. Radiation Physics and Chemistry, 2013, 85, 59-63.	1.4	16
107	The d-electrons of Fe in ferrocene: the excess orbital energy spectrum (EOES). RSC Advances, 2015, 5, 11933-11941.	1.7	16
108	Two conformers of a tyrosine kinase inhibitor (AG-1478) disclosed using simulated UV-Vis absorption spectroscopy. New Journal of Chemistry, 2016, 40, 8296-8304.	1.4	16

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109	Enhanced photocatalytic activity of g-C3N4/MnO composites for hydrogen evolution under visible light. Dalton Transactions, 2019, 48, 14864-14872.	1.6	16
110	Variational calculation of the ro-vibrational states of Na3+. Molecular Physics, 1992, 77, 1197-1207.	0.8	15
111	Prediction of spectroscopic constants for diatomic molecules in the ground and excited states using time-dependent density functional theory. Journal of Computational Chemistry, 2006, 27, 163-173.	1.5	15
112	Throughput based temporal verification for monitoring large batch of parallel processes. , 2014, , .		15
113	Microporous organic polymers based on tetraethynyl building blocks with N-functionalized pore surfaces: synthesis, porosity and carbon dioxide sorption. RSC Advances, 2016, 6, 113826-113833.	1.7	15
114	Synthesis and photovoltaic properties of donorâ€“acceptor conjugated polymers based on 4,7-dithienyl-2,1,3-benzothiadiazole functionalized silole. Synthetic Metals, 2016, 220, 433-439.	2.1	15
115	Element-free Galerkin scaled boundary method based on moving Kriging interpolation for steady heat conduction analysis. Engineering Analysis With Boundary Elements, 2019, 106, 440-451.	2.0	15
116	Variational calculations of rotationally resolved infrared properties of Li2Na+, LiNa2+ and KLiNa+. Journal of Molecular Structure, 1992, 272, 73-93.	1.8	14
117	Potential energy surface for and pure rotational spectra of isotopomeric Cl2â€“Ar van der Waals complexes. Journal of Chemical Physics, 1996, 104, 9304-9312.	1.2	14
118	Core molecular orbital contribution to N2O isomerization as studied using theoretical electron momentum spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 9-15.	2.0	14
119	A high-resolution electron momentum spectroscopy and density functional theory study into the complete valence electronic structure of allene. Journal of Computational Chemistry, 2001, 22, 1321-1333.	1.5	14
120	Molecular orbitals of methane: symmetry or hybridization?. Computational and Theoretical Chemistry, 2004, 678, 105-111.	1.5	14
121	Valence space electron momentum spectroscopy of diborane. Journal of Electron Spectroscopy and Related Phenomena, 2006, 151, 215-223.	0.8	14
122	Solvent effects on blue shifted improper hydrogen bond of Câ€“Hâ‹¯O in deoxycytidine isomers. Chemical Physics Letters, 2010, 500, 327-333.	1.2	14
123	Electron shell contributions to gamma-ray spectra of positron annihilation in noble gases. Journal of Physics B: Atomic, Molecular and Optical Physics, 2010, 43, 165207.	0.6	14
124	Photoelectron Spectra of Some Antibiotic Building Blocks: 2-Azetidinone and Thiazolidine-Carboxylic Acid. Journal of Physical Chemistry A, 2012, 116, 8653-8660.	1.1	14
125	Chemical structural effects on Î³-ray spectra of positron annihilation in fluorobenzenes. European Physical Journal D, 2012, 66, 1.	0.6	14
126	Effects of quantum chemistry models for bound electrons on positron annihilation spectra for atoms and small molecules. New Journal of Physics, 2012, 14, 085022.	1.2	14

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127	UVâ€“Vis spectroscopy and solvatochromism of the tyrosine kinase inhibitor AG-1478. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 164, 128-132.	2.0	14
128	Investigation of adsorption, dissociation, and diffusion properties of hydrogen on the V (1â€¯0â€¯0) surface and in the bulk: A first-principles calculation. Journal of Advanced Research, 2020, 21, 25-34.	4.4	14
129	The importance of the molecular weight of PEDOT hole transporting materials for efficient organic solar cells. Journal of Materials Chemistry C, 2020, 8, 17185-17193.	2.7	14
130	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
131	Use of simulated infrared spectra to test N2-Ar pair potentials and dipole moment surfaces. Molecular Physics, 1996, 88, 821-840.	0.8	14
132	Chemical bonding mechanisms of n-butane probed by the core orbitals of conformational isomers in r-space and k-space. Chemical Physics Letters, 2004, 384, 144-149.	1.2	13
133	Impact of ketone and amino on the inner shell ofÂguanine. Journal of Synchrotron Radiation, 2009, 16, 545-552.	1.0	13
134	Density Functional Study on Core Ionization Spectra of Cytidine and Its Fragments. Bulletin of the Chemical Society of Japan, 2009, 82, 187-195.	2.0	13
135	In Silico Investigation of Lactone and Thiolactone Inhibitors in Bacterial Quorum Sensing Using Molecular Modeling. International Journal of Chemistry, 2013, 5, .	0.3	13
136	Ferrocene Orientation Determined Intramolecular Interactions Using Energy Decomposition Analysis. Materials, 2015, 8, 7723-7737.	1.3	13
137	Conformation Analysis of Ferrocene and Decamethylferrocene via Full-Potential Modeling of XANES and XAFS Spectra. Journal of Physical Chemistry Letters, 2016, 7, 2792-2796.	2.1	13
138	Reinterpretation of Dynamic Vibrational Spectroscopy to Determine the Molecular Structure and Dynamics of Ferrocene. Chemistry - A European Journal, 2016, 22, 18019-18026.	1.7	13
139	Electronic structure and intramolecular interactions in three methoxyphenol isomers. Journal of Chemical Physics, 2018, 149, 134312.	1.2	13
140	Insights into the dissociative ionization of glycine by PEPICO experiments. Physical Chemistry Chemical Physics, 2018, 20, 22841-22848.	1.3	13
141	The electronic structure of small lithium clusters. Journal of Cluster Science, 1991, 2, 203-217.	1.7	12
142	Ab initio calculations of the rotationally resolved infrared spectrum of KNa 2 +. Theoretica Chimica Acta, 1994, 88, 131-145.	0.9	12
143	An electron momentum spectroscopy and density functional theory investigation into the complete valence electronic structure of ethylene oxide. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 3239-3253.	0.6	12
144	An (e,2e) coincidence study of formic acid monomer and dimer. Chemical Physics Letters, 2008, 451, 18-24.	1.2	12

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145	Differentiation of alkane isomers through binding energy spectra and total momentum cross sections. New Journal of Chemistry, 2014, 38, 1031.	1.4	12
146	Molecular dynamics studies on the NMR structures of rabbit prion protein wild type and mutants: surface electrostatic charge distributions. Journal of Biomolecular Structure and Dynamics, 2015, 33, 1326-1335.	2.0	12
147	Novel 4,5-diazafluorene-based Schiff base derivatives as Al 3+ ions fluorescence turn-on sensors. Synthetic Metals, 2016, 217, 37-42.	2.1	12
148	Hypercrosslinked siloleâ€containing microporous organic polymers with <scp>N</scp>â€functionalized pore surfaces for gas storage and separation. Journal of Applied Polymer Science, 2018, 135, 45907.	1.3	12
149	Differentiation of adenine non-planarity in valence molecular orbitals. Molecular Simulation, 2006, 32, 667-673.	0.9	11
150	Docking Positrophilic Electrons into Molecular Attractive Potentials of Fluorinated Methanes. Journal of the Physical Society of Japan, 2013, 82, 104301.	0.7	11
151	Synthesis of Ï€-Extended Dithienobenzodithiophene-Containing Medium Bandgap Copolymers and Their Photovoltaic Application. Journal of Macromolecular Science - Pure and Applied Chemistry, 2015, 52, 934-941.	1.2	11
152	Synthesis and Photovoltaic Properties of 2D-Conjugated Polymers Based on Alkylthiothienyl-Substituted Benzodithiophene and Different Accepting Units. Polymers, 2018, 10, 331.	2.0	11
153	Valence Orbital Electron Momentum Spectroscopy For N2O. Journal of Physical Chemistry A, 2001, 105, 1254-1259.	1.1	10
154	Intramolecular proton transfer in adenine imino tautomers. Molecular Simulation, 2006, 32, 1261-1270.	0.9	10
155	Effects of alkyl side chains on properties of aliphatic amino acids probed using quantum chemical calculations. Journal of Synchrotron Radiation, 2011, 18, 733-742.	1.0	10
156	Density functional study of Cu2+-phenylalanine complex under micro-solvation environment. Journal of Molecular Graphics and Modelling, 2013, 45, 180-191.	1.3	10
157	Rational use of ligand to shift the UVâ€“vis spectrum of Ru-complex sensitiser dyes for DSSC applications. Radiation Physics and Chemistry, 2019, 161, 66-71.	1.4	10
158	Radiation Damage Mechanisms of Chemotherapeutically Active Nitroimidazole Derived Compounds. Frontiers in Chemistry, 2019, 7, 329.	1.8	10
159	Variational calculations of rovibrational states of Li2K+. Chemical Physics, 1993, 172, 247-258.	0.9	9
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