

Weizhou Wang

List of Publications by Year in descending order

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96
papers

3,407
citations

159585

30
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149698

56
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99
all docs

99
docs citations

99
times ranked

3606
citing authors

#	ARTICLE	IF	CITATIONS
1	Chalcogen Bond: A Sister Noncovalent Bond to Halogen Bond. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8132-8135.	2.5	489
2	Ïƒ-Hole Bond vs Ïƒ-Hole Bond: A Comparison Based on Halogen Bond. <i>Chemical Reviews</i> , 2016, 116, 5072-5104.	47.7	487
3	Theoretical Study on the Blueshifting Halogen Bond. <i>Journal of Physical Chemistry A</i> , 2004, 108, 1799-1805.	2.5	186
4	Origin of the X ^{δ-} Hal (Hal = Cl, Br) Bond-Length Change in the Halogen-Bonded Complexes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4114-4119.	2.5	115
5	Halogen bonding in room-temperature phosphorescent materials. <i>Coordination Chemistry Reviews</i> , 2020, 404, 213107.	18.8	106
6	Noncovalent Ïƒ ^π ... π ...Ïƒ interaction between graphene and aromatic molecule: Structure, energy, and nature. <i>Journal of Chemical Physics</i> , 2014, 140, 094302.	3.0	83
7	Sub-5 nm Monolayer Arsenene and Antimonene Transistors. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 22363-22371.	8.0	77
8	Symmetrical Bifurcated Halogen Bond: Design and Synthesis. <i>Crystal Growth and Design</i> , 2011, 11, 3622-3628.	3.0	74
9	Structures, mobility and electronic properties of point defects in arsenene, antimonene and an antimony arsenide alloy. <i>Journal of Materials Chemistry C</i> , 2017, 5, 4159-4166.	5.5	72
10	Synthesis, Structure, and Photophysical Properties of Two Four-Coordinate Cu ^I â€“NHC Complexes with Efficient Delayed Fluorescence. <i>Inorganic Chemistry</i> , 2016, 55, 2157-2164.	4.0	70
11	C ₁₂ H Stretching Vibrational Shift of Benzene Dimer: Consistency of Experiment and Calculation. <i>ChemPhysChem</i> , 2007, 8, 2107-2111.	2.1	67
12	Theoretical Study on the Complexes of Benzene with Isoelectronic Nitrogenâ€“Containing Heterocycles. <i>ChemPhysChem</i> , 2008, 9, 1003-1009.	2.1	64
13	Syntheses, Structures, Luminescence, and Magnetic Properties of One-dimensional Lanthanide Coordination Polymers with a Rigid 2,2â€“Bipyridine-3,3â€“,6,6â€“-tetracarboxylic Acid Ligand. <i>Inorganic Chemistry</i> , 2012, 51, 2170-2177.	4.0	64
14	Phosphorescent Ïƒ-Hole- π -Ïƒ Bonding Cocrystals of Pyrene with Halo-perfluorobenzenes (F, Cl, Br, I). <i>Crystal Growth and Design</i> , 2015, 15, 4938-4945.	3.0	62
15	Some theoretical observations on the 1:1 glycine zwitterionâ€“water complex. <i>Computational and Theoretical Chemistry</i> , 2003, 626, 127-132.	1.5	55
16	Halogen Bond Involving Hypervalent Halogen: CSD Search and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 9294-9299.	2.5	55
17	On the Difference of the Properties between the Blue-Shifting Halogen Bond and the Blue-Shifting Hydrogen Bond. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7257-7260.	2.5	47
18	Theoretical Study of 1,3,4,6,7,9,9b-Heptaazaphenalene and Its Ten Derivatives. <i>Journal of Physical Chemistry A</i> , 2004, 108, 97-106.	2.5	46

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19	Prolylprolinolâ€Catalyzed Asymmetric Michael Addition of Aliphatic Aldehydes to Nitroalkenes. <i>Advanced Synthesis and Catalysis</i> , 2010, 352, 644-650.	4.3	45
20	The Nature of the Noncovalent Interactions between Benzene and C ₆₀ Fullerene. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5766-5772.	2.5	41
21	Theoretical Study on the Bromomethaneâ€Water 1:2 Complexes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8035-8040.	2.5	40
22	Interactions between haloperfluorobenzenes and fluoranthene in luminescent cocrystals from Î€-holeâ€Î€ to Îƒ-holeâ€Î€ bonds. <i>CrystEngComm</i> , 2017, 19, 5058-5067.	2.6	40
23	A Twoâ€Step Sequence to Ethyl Î±â€Fluorocyclopropanecarboxylates Through MIRC Reaction of Ethyl Dichloroacetate and Highly Regioselective Fluorination. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 7372-7381.	2.4	39
24	Performance Limit of Monolayer WSe ₂ Transistors; Significantly Outperform Their MoS ₂ Counterpart. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 20633-20644.	8.0	39
25	Novel pyrene derivatives: Synthesis, properties and highly efficient non-doped deep-blue electroluminescent device. <i>Dyes and Pigments</i> , 2012, 92, 732-736.	3.7	35
26	The 1:1 glycineâ€water complex: some theoretical observations. <i>Computational and Theoretical Chemistry</i> , 2002, 618, 235-244.	1.5	34
27	Structural Competition between Halogen Bonds and Loneâ€Pairâ€â€â€ Interactions in Solution. <i>ChemPhysChem</i> , 2012, 13, 1411-1414.	2.1	34
28	Communication: Competition between <i>Î€</i>â€<i>Î€</i> interaction and halogen bond in solution: A combined 13C NMR and density functional theory study. <i>Journal of Chemical Physics</i> , 2012, 136, 141101.	3.0	33
29	On the correlation between bond-length change and vibrational frequency shift in halogen-bonded complexes. <i>Journal of Chemical Physics</i> , 2011, 134, 224303.	3.0	32
30	Performance limit of monolayer MoSi ₂ N ₄ transistors. <i>Journal of Materials Chemistry C</i> , 2021, 9, 14683-14698.	5.5	32
31	A new class of halogen bonds that avoids the Îƒ-hole. <i>Chemical Physics Letters</i> , 2012, 532, 27-30.	2.6	31
32	Intermolecular and very strong intramolecular Câ€Seâ€O/N chalcogen bonds in nitrophenyl selenocyanate crystals. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 5227-5234.	2.8	28
33	Hyperconjugation versus intramolecular hydrogen bond: origin of the conformational preference of gaseous glycine. <i>Chemical Physics Letters</i> , 2003, 370, 147-153.	2.6	26
34	Determination of cis-diol-containing flavonoids in real samples using boronate affinity quantum dots coated with imprinted silica based on controllable oriented surface imprinting approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 227, 117542.	3.9	26
35	Effects of functional groups for CO ₂ capture using metal organic frameworks. <i>Frontiers of Chemical Science and Engineering</i> , 2021, 15, 437-449.	4.4	26
36	The benzeneâ€naphthalene complex: A more challenging system than the benzene dimer for newly developed computational methods. <i>Journal of Chemical Physics</i> , 2015, 143, 114312.	3.0	24

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37	Solubility Measurement and the Correlation of 1-Naphthaleneacetic Acid in Pure and Methanol + Water Binary Solvents from $T = (278.25 \text{ to } 323.55) \text{ K}$. <i>Journal of Chemical & Engineering Data</i> , 2017, 62, 1292-1301.	1.9	24
38	Highly accurate benchmark calculations of the interaction energies in the complexes $C_6H_6 \cdot \cdot C_6X_6$ ($X = F, Cl, Br, \text{ and } I$). <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25345.	2.0	24
39	Zinc 2-N-methyl N-confused porphyrin: an efficient catalyst for the conversion of CO_2 into cyclic carbonates. <i>Catalysis Science and Technology</i> , 2019, 9, 4255-4261.	4.1	24
40	Benchmark calculations of the adsorption of aromatic molecules on graphene. <i>Journal of Computational Chemistry</i> , 2015, 36, 1763-1771.	3.3	23
41	The $\pi\text{-}\pi$ Stacking Interactions between Homogeneous Dimers of $C_6F_xI(6-x)$ ($x = 0, 1, 2, 3, 4, \text{ and } 5$): A Comparative Study with the Halogen Bond. <i>Journal of Physical Chemistry A</i> , 2012, 116, 12486-12491.	2.5	21
42	Tetrel bonding on graphene. <i>Computational and Theoretical Chemistry</i> , 2019, 1147, 8-12.	2.5	21
43	Structural competition between $\pi\text{-}\pi$ interactions and halogen bonds: a crystallographic study. <i>CrystEngComm</i> , 2013, 15, 769-774.	2.6	20
44	Substituent effects in the $\pi\text{-}\pi$ interaction between graphene and benzene: An indication for the noncovalent functionalization of graphene. <i>Computational and Theoretical Chemistry</i> , 2014, 1046, 64-69.	2.5	19
45	Hydrogen bond and halogen bond inside the carbon nanotube. <i>Journal of Chemical Physics</i> , 2011, 134, 054317.	3.0	18
46	Effect of carboxylic acid on micelles of a neutral amphiphilic dendro-calix[4]arene. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 729-735.	2.8	18
47	Prediction of a Family of Cage-shaped Boric Acid Clusters. <i>Journal of Physical Chemistry B</i> , 2005, 109, 8562-8564.	2.6	17
48	Metal-Organic Frameworks Grafted by Univariate and Multivariate Heterocycles for Enhancing CO_2 Capture: A Molecular Simulation Study. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 2195-2205.	3.7	17
49	Self-curl and self-assembly of boric acid clusters. <i>Chemical Physics Letters</i> , 2005, 405, 425-428.	2.6	16
50	The bifurcate chalcogen bond: Some theoretical observations. <i>Computational and Theoretical Chemistry</i> , 2009, 916, 135-138.	1.5	16
51	The Existence of a $N \rightarrow C$ Dative Bond in the $C_6H_6 \cdot \cdot$ Piperidine Complex. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 1942-1950.	13.8	15
52	Unconventional interaction in N(P)-related systems. <i>Chemical Physics Letters</i> , 2005, 411, 439-444.	2.6	14
53	Pseudo-Bifurcated Chalcogen Bond in Crystal Engineering. <i>Crystals</i> , 2018, 8, 163.	2.2	14
54	The $\pi\text{-}\pi$ hole-hole stacking interaction: An unrecognized type of noncovalent interaction. <i>Journal of Chemical Physics</i> , 2020, 153, 214302.	3.0	14

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55	Determination and Correlation of Solubilities of 2-Isopropylthioxanthone (ITX) in Seven Different Solvents from (299.15 to 329.85) K. <i>Journal of Chemical & Engineering Data</i> , 2015, 60, 941-946.	1.9	13
56	Highly efficient undoped deep-blue electroluminescent device based on a novel pyrene derivative. <i>Solid-State Electronics</i> , 2010, 54, 524-526.	1.4	12
57	ASSESSMENT OF THE PERFORMANCE OF THE M05-CLASS AND M06-CLASS FUNCTIONALS FOR THE STRUCTURE AND GEOMETRY OF THE HYDROGEN-BONDED AND HALOGEN-BONDED COMPLEXES. <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 1165-1173.	1.8	12
58	Unexpected strong stacking interactions between the homogeneous dimers of C ₆ F _x I(6- ^x) (x=0, 1, 2, 3, 4) Tj ETQ _{0,0} 0 rgBTJ/Overlock	2.5	12
59	Improper halogen bond in the crystal structure. <i>CrystEngComm</i> , 2013, 15, 3093.	2.6	12
60	The nature of the noncovalent interactions between fullerene C ₆₀ and aromatic hydrocarbons. <i>Computational and Theoretical Chemistry</i> , 2017, 1122, 34-39.	2.5	12
61	Ab Initio Study of Gas Adsorption in Metal-Organic Frameworks Modified by Lithium: The Significant Role of Li-Containing Functional Groups. <i>Journal of Physical Chemistry C</i> , 2018, 122, 18395-18404.	3.1	11
62	Toward a less costly but accurate calculation of the CCSD(T)/CBS noncovalent interaction energy. <i>Journal of Computational Chemistry</i> , 2020, 41, 1252-1260.	3.3	11
63	Application of Berlin's Theorem to Bond-Length Changes in Isolated Molecules and Red- and Blue-Shifting H-Bonded Clusters. <i>Collection of Czechoslovak Chemical Communications</i> , 2008, 73, 862-872.	1.0	10
64	A theoretical study of the atomic hydrogen binding on small Ag Cu (n+m=5) clusters. <i>Computational and Theoretical Chemistry</i> , 2010, 959, 75-79.	1.5	10
65	The nature of the π interactions and a comparative study with the nature of the π interactions. <i>Computational and Theoretical Chemistry</i> , 2014, 1030, 1-8.	2.5	10
66	An ab initio study of P-H interactions using the PH ₃ -PH ₃ model complex. <i>Computational and Theoretical Chemistry</i> , 2003, 625, 25-30.	1.5	9
67	Method-dependent relative stability of hydrogen bonded and π stacked structures of the formic acid tetramer. <i>Chemical Physics Letters</i> , 2005, 402, 54-56.	2.6	9
68	Strength order and nature of the π -hole bond of cyanuric chloride and 1,3,5-triazine with halide. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 20636-20646.	2.8	9
69	On the nature of the stacking interaction between two graphene layers. <i>Chemical Physics Letters</i> , 2015, 620, 46-49.	2.6	9
70	Structure-directed formation of the dative/covalent bonds in complexes with C ₇₀ -piperidine. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4365-4375.	2.8	9
71	The nature of the bond-length change upon molecule complexation. <i>Collection of Czechoslovak Chemical Communications</i> , 2010, 75, 243-256.	1.0	7
72	Theoretical rationale for the role of the strong halogen bond in the design and synthesis of organic semiconductor materials. <i>Computational and Theoretical Chemistry</i> , 2021, 1194, 113074.	2.5	7

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73	Computational screening of heterocycle decorations in metal-organic frameworks for efficient C2/C1 adsorption and separation. <i>Fuel</i> , 2020, 279, 118431.	6.4	6
74	Addition Reaction between Piperidine and C ₆₀ to Form 1,4-Disubstituted C ₆₀ Proceeds through van der Waals and Dative Bond Complexes: Theoretical and Experimental Study. <i>Journal of the American Chemical Society</i> , 2021, 143, 10930-10939.	13.7	6
75	A Robust Supramolecular Heterosynthron Assembled by a Hydrogen Bond and a Chalcogen Bond. <i>Crystals</i> , 2021, 11, 1309.	2.2	6
76	Noncovalent Interactions between 1,3,5-Trifluoro-2,4,6-triiodobenzene and a Series of 1,10-Phenanthroline Derivatives: A Combined Theoretical and Experimental Study. <i>Crystals</i> , 2019, 9, 140.	2.2	5
77	Accurate calculations of the noncovalent systems with flat potential energy surfaces: Naphthalene dimer and azulene dimer. <i>Computational and Theoretical Chemistry</i> , 2017, 1112, 52-60.	2.5	4
78	Weakening and Leveling Effect of Solvent Polarity on Halogen Bond Strength of Diiodoperfluoroalkane with Halide. <i>Journal of Solution Chemistry</i> , 2017, 46, 1092-1103.	1.2	4
79	Supramolecular Interactions of Fullerene C ₆₀ with 1,3,5-Trifluoro-2,4,6-triiodobenzene: A Combined Theoretical and Experimental Study. <i>ChemPlusChem</i> , 2018, 83, 470-477.	2.8	4
80	Unexpected Sandwiched-Layer Structure of the Cocrystal Formed by Hexamethylbenzene with 1,3-Diiodotetrafluorobenzene: A Combined Theoretical and Crystallographic Study. <i>Crystals</i> , 2020, 10, 379.	2.2	4
81	The Existence of a N ⁺ C Dative Bond in the C ₆₀ –Piperidine Complex. <i>Angewandte Chemie</i> , 2021, 133, 1970-1978.	2.0	4
82	Effect of CP-corrected gradient optimization on the water-radical (anion) dimer hypersurface. <i>Computational and Theoretical Chemistry</i> , 2003, 631, 171-180.	1.5	3
83	Thioformyl chloride dimer: An excellent model system for the assessment of new computational methods. <i>Computational and Theoretical Chemistry</i> , 2012, 983, 83-87.	2.5	2
84	Structural study on four co-crystals of N-containing heteroaromatics with iodofluorobenzene. <i>Chemical Research in Chinese Universities</i> , 2015, 31, 84-90.	2.6	2
85	Crystal structure of halogen-bonded 2-chloro-1,10-phenanthroline–1,4-diiodotetrafluorobenzene (2/1), C ₃₀ H ₁₄ Cl ₂ F ₄ I ₂ N ₄ . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2017, 232, 323-324.	0.3	2
86	Determination and Correlation of Solubilities of 1,3,5-Trifluoro-2,4,6-triiodobenzene in Different Solvents from 289.25 to 332.15 K. <i>Journal of Chemical & Engineering Data</i> , 2019, 64, 4306-4313.	1.9	2
87	Halogen bonds in the crystal structure of 4,3:5,4-terpyridine – 1,4-diiodotetrafluorobenzene (1/1), C ₂₁ H ₁₁ F ₄ I ₂ N ₃ . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2019, 234, 935-937.	0.3	2
88	The Face-to-Face ĩf-Hole–ĩf-Hole Stacking Interactions: Structures, Energies, and Nature. <i>Crystals</i> , 2021, 11, 877.	2.2	2
89	The Bifurcated ĩf-Hole–ĩf-Hole Stacking Interactions. <i>Molecules</i> , 2022, 27, 1252.	3.8	2
90	SN ₂ -like Reaction in Hydrogen-Bonded Complexes: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9353-9355.	2.5	1

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91	Halogen bonds and $\pi\cdots\pi$ interactions in the crystal structure of 1,3,5-trifluoro-2,4,6-triiodobenzene \cdot <i>N,N</i> -dimethylformamide (1/1), C ₉ H ₇ F ₃ I ₃ NO. Zeitschrift Fur Kristallographie - New Crystal Structures, 2017, 232, 937-938.	0.3	1
92	Halogen bonds in the crystal structure of 5-bromo-3,4-bipyridine \cdot 1,4-diiodotetrafluorobenzene (2/1), C ₂₆ H ₁₄ Br ₂ F ₄ I ₂ N ₄ . Zeitschrift Fur Kristallographie - New Crystal Structures, 2019, 234, 1187-1188.	0.3	1
93	Origin of the unexpected attractive interactions between positive π -holes and positive π -lumps. Computational and Theoretical Chemistry, 2022, 1213, 113736.	2.5	1
94	Crystal structure of 2,9-dibromo-1,10-phenanthroline, C ₁₂ H ₆ Br ₂ N ₂ . Zeitschrift Fur Kristallographie - New Crystal Structures, 2017, 232, 441-442.	0.3	0
95	Halogen bonds in the crystal structure of 4,3,5-terpyridine \cdot 1,3-diiodotetrafluorobenzene (1/1), C ₂₁ H ₁₁ F ₄ I ₂ N ₃ . Zeitschrift Fur Kristallographie - New Crystal Structures, 2022, 237, 161-163.	0.3	0
96	Chalcogen bonds in the crystal structure of 4,7-dibromo-2,1,3-benzoselenadiazole, C ₆ H ₂ Br ₂ N ₂ Se. Zeitschrift Fur Kristallographie - New Crystal Structures, 2022, 237, 169-171.	0.3	0