

Hui-Li Xu

List of Publications by Year in descending order

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papers

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#	ARTICLE	IF	CITATIONS
1	Monolayer TiO_2 : A Promising Candidate for NH_3 Sensor or Capturer with High Sensitivity and Selectivity. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 13707-13713.	8.0	524
2	The Role of Methyl Groups in the Formation of Hydrogen Bond in DMSO-Methanol Mixtures. <i>Journal of the American Chemical Society</i> , 2006, 128, 1438-1439.	13.7	183
3	Cooperativity between the Halogen Bond and the Hydrogen Bond in $\text{H}_3\text{N}^+\cdots\text{XY}^-\cdots\text{HF}$ Complexes (X, Y=F, Cl, Br). <i>ChemPhysChem</i> , 2008, 9, 2265-2269.	2.1	152
4	Concerted Interaction between Pnictogen and Halogen Bonds in $\text{XCl}_2\text{FH}_2\text{PNH}_3$ (X=F, OH, CN, NC, and FCC). <i>ChemPhysChem</i> , 2012, 13, 1205-1212.	2.1	124
5	A π -hole interaction with radical species as electron donors: does single-electron tetrel bonding exist?. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 11617-11625.	2.8	113
6	Excess Infrared Absorption Spectroscopy and its Applications in the Studies of Hydrogen Bonds in Alcohol-Containing Binary Mixtures. <i>Applied Spectroscopy</i> , 2008, 62, 166-170.	2.2	109
7	Competition and cooperativity between tetrel bond and chalcogen bond in complexes involving F_2CX (X = Se and Te). <i>Chemical Physics Letters</i> , 2015, 620, 7-12.	2.6	103
8	Comparison of tetrel bonds in neutral and protonated complexes of pyridine and furan with NH_3 (T = C, Si, and Ge). <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 5550-5559.	2.8	98
9	A bioinspired hybrid membrane with wettability and topology anisotropy for highly efficient fog collection. <i>Journal of Materials Chemistry A</i> , 2019, 7, 124-132.	10.3	93
10	Competition between hydrogen bond and halogen bond in complexes of formaldehyde with hypohalous acids. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6837.	2.8	92
11	The band gap modulation of monolayer TiO_2 by strain. <i>RSC Advances</i> , 2015, 5, 30438-30444.	3.6	82
12	Highly selective and sensitive turn-on fluorescent sensor for detection of Al^{3+} based on quinoline-base Schiff base. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 195, 157-164.	3.9	82
13	Cooperativity between $\text{OH}\cdots\text{O}$ and $\text{CH}\cdots\text{O}$ Hydrogen Bonds Involving Dimethyl Sulfoxide- H_2O Complex. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10166-10169.	2.5	81
14	Tetrel-Hydride Interaction between XH_3F (X = C, Si, Ge, Sn) and HM (M = Li, Na, BeH, MgH). <i>Journal of Physical Chemistry A</i> , 2015, 119, 2217-2224.	2.5	79
15	Pnictogen-Hydride Interaction between FH_2X (X = P and As) and HM (M = ZnH, BeH, MgH, Li). <i>Tj ETQq1 1 0.784314 rgBT</i>	2.5	75
16	Competition of chalcogen bond, halogen bond, and hydrogen bond in SCSHOX and SeCSeHOX (X=Cl) <i>Tj ETQq0 0 0 rgBT /Overlock 10 T</i>	2.5	72
17	Comparative Strengths of Tetrel, Pnictogen, Chalcogen, and Halogen Bonds and Contributing Factors. <i>Molecules</i> , 2018, 23, 1681.	3.8	69
18	Tetrel bond of pseudohalide anions with XH_3F (X = C, Si, Ge, and Sn) and its role in SN_2 reaction. <i>Journal of Chemical Physics</i> , 2016, 145, 224310.	3.0	68

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19	Some measures for making halogen bonds stronger than hydrogen bonds in $H_2CS=HOX$ ($X = F, Cl, Br, I$) complexes. <i>Journal of Chemical Physics</i> , 2009, 128, 104314.	2.8	66
20	Prediction and characterization of the $HMgH^{\ominus}LiX$ ($X = H, OH, F, CCH, CN, \text{ and } NC$) complexes: a lithium-hydride lithium bond. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 2402.	2.8	64
21	Interplay between halogen bond and lithium bond in $MCN^{\ominus}LiCN^{\ominus}XCCH$ ($M = H, Li, \text{ and } Na; X = Cl, Br, \text{ and } I$) complex: The enhancement of halogen bond by a lithium bond. <i>Journal of Computational Chemistry</i> , 2011, 32, 3296-3303.	3.3	61
22	A high performance 2-hydroxynaphthalene Schiff base fluorescent chemosensor for Al^{3+} and its applications in imaging of living cells and zebrafish in vivo. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 207, 31-38.	3.9	60
23	An unconventional halogen bond with carbene as an electron donor: An ab initio study. <i>Chemical Physics Letters</i> , 2009, 469, 48-51.	2.6	58
24	Resveratrol Ameliorates Diabetes-Induced Cardiac Dysfunction Through $AT1R$ -ERK/p38 MAPK Signaling Pathway. <i>Cardiovascular Toxicology</i> , 2016, 16, 130-137.	2.7	57
25	Cooperativity between two types of hydrogen bond in $H_3C^{\ominus}HCN^{\ominus}HCN$ and $H_3C^{\ominus}HNC^{\ominus}HNC$ complexes. <i>Journal of Chemical Physics</i> , 2008, 128, 154102.	3.0	56
26	Substitution, cooperative, and solvent effects on π -pnictogen bonds in the FH_2P and FH_2As complexes. <i>Journal of Molecular Modeling</i> , 2012, 18, 4325-4332.	1.8	56
27	Interplay between tetrel bonding and hydrogen bonding interactions in complexes involving F_2XO ($X = C \text{ and } Si$) and HCN . <i>Computational and Theoretical Chemistry</i> , 2014, 1050, 51-57.	2.5	55
28	Influence of Substitution, Hybridization, and Solvent on the Properties of $C\dot{\ominus}HO$ Single-Electron Hydrogen Bond in $CH_3^{\oplus}H_2O$ Complex. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5258-5263.	2.5	53
29	A dual functional turn-on non-toxic chemosensor for highly selective and sensitive visual detection of Mg^{2+} and Zn^{2+} : the solvent-controlled recognition effect and bio-imaging application. <i>Analyst</i> , 2019, 144, 4024-4032.	3.5	53
30	The development of coumarin Schiff base system applied as highly selective fluorescent/colorimetric probes for Cu^{2+} and tumor biomarker glutathione detection. <i>Dyes and Pigments</i> , 2020, 175, 108156.	3.7	51
31	Cooperativity between the Dihydrogen Bond and the $N\dot{\ominus}\dots\dot{\ominus}HC$ Hydrogen Bond in $LiH^{\ominus}(HCN)_n$ Complexes. <i>ChemPhysChem</i> , 2008, 9, 1942-1946.	2.1	47
32	Spectroscopic and theoretical evidence for the cooperativity between red-shift hydrogen bond and blue-shift hydrogen bond in DMSO aqueous solutions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 69, 211-215.	3.9	47
33	Carbene tetrel-bonded complexes. <i>Structural Chemistry</i> , 2017, 28, 823-831.	2.0	47
34	The π -tetrel Bond and its Influence on Hydrogen Bonding and Proton Transfer. <i>ChemPhysChem</i> , 2018, 19, 736-743.	2.1	46
35	Regulating Function of Methyl Group in Strength of $CH_3^{\oplus}\dot{\ominus}O$ Hydrogen Bond: A High-Level Ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3985-3990.	2.5	45
36	$Se^{\oplus}\dot{\ominus}N$ Chalcogen Bond and $Se^{\oplus}\dot{\ominus}X$ Halogen Bond Involving $F_2C^{\oplus}Se$: Influence of Hybridization, Substitution, and Cooperativity. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3518-3527.	2.5	45

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37	Carbon Excess C ₃ N: A Potential Candidate as Li-Ion Battery Material. ACS Applied Materials & Interfaces, 2018, 10, 37135-37141.	8.0	44
38	Ab Initio Study of Lithium-Bonded Complexes with Carbene as an Electron Donor. Journal of Physical Chemistry A, 2009, 113, 14156-14160.	2.5	43
39	The Prominent Enhancing Effect of the Cation-π Interaction on the Halogen-Hydride Halogen Bond in M ⁺ ...C ₆ H ₅ X...HM ²⁺ . ChemPhysChem, 2011, 12, 2289-2295.	2.1	41
40	Cooperative and Diminutive Effects of Pnictogen Bonds and Cation-π Interactions. ChemPhysChem, 2014, 15, 500-506.	2.1	38
41	Comparison of σ-Hole and π-Hole Tetrel Bonds Formed by Pyrazine and 1,4-Dicyanobenzene: The Interplay between Anion-π and Tetrel Bonds. ChemPhysChem, 2017, 18, 2442-2450.	2.1	38
42	Tetrel bonds between PySiX ₃ and some nitrogenated bases: Hybridization, substitution, and cooperativity. Journal of Molecular Graphics and Modelling, 2016, 65, 35-42.	2.4	36
43	Prominent Effect of Alkali Metals in Halogen-Bonded Complex of MCCBr ⁺ NCM ²⁺ (M and M ²⁺ = H, Li, Na, F). Tj ETOq1 1 0,784314 g	2.5	34
44	Complexes between hypohalous acids and phosphine derivatives. Pnictogen bond versus halogen bond versus hydrogen bond. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 132, 271-277.	3.9	33
45	The aerogen-π bonds involving π systems. Chemical Physics Letters, 2016, 651, 50-55.	2.6	33
46	Cooperative effects between π-hole triel and π-hole chalcogen bonds. RSC Advances, 2018, 8, 26580-26588.	3.6	33
47	Ab initio study of the cooperativity between NH ₃ and NH ₃ hydrogen bonds in H ₃ N ⁺ ...HNC ⁻ ...HNC complex. Theoretical Chemistry Accounts, 2010, 127, 303-309.	1.4	32
48	Competition and cooperativity between hydrogen bond and halogen bond in HNC ⁻ (HOBr) _n and (HNC) _n ...HOBr (n=1 and 2) systems. Computational and Theoretical Chemistry, 2011, 963, 417-421.	2.5	31
49	Prediction and characterization of a chalcogen-hydride interaction with metal hybrids as an electron donor in F ₂ CS ⁺ HM and F ₂ CSe ⁺ HM (M = Li, Na, BeH, MgH, MgCH ₃) complexes. Physical Chemistry Chemical Physics, 2012, 14, 3025.	2.8	31
50	Highly selective and sensitive chemosensor for Al(III) based on isoquinoline Schiff base. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 243, 118754.	3.9	31
51	Is π halogen bonding or lone pair-π interaction formed between borazine and some halogenated compounds?. Physical Chemistry Chemical Physics, 2014, 16, 159-165.	2.8	30
52	Surprising enhancing effect of methyl group on the strength of O...XF and S...XF (X=Cl and Br) halogen bonds. Journal of Chemical Physics, 2010, 133, 114303.	3.0	29
53	Halogen bonds with N-heterocyclic carbenes as halogen acceptors: a partially covalent character. Molecular Physics, 2014, 112, 3024-3032.	1.7	29
54	Theoretical study of the cooperative effects between the triel bond and the pnictogen bond in BF ₃ ...NCXH ₂ ...Y (X = P, As, Sb; Y = H ₂ O, NH ₃) complexes. Journal of Molecular Modeling, 2016, 22, 10.	1.8	29

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55	Cooperative and substitution effects in enhancing strengths of halogen bonds in FCl $\hat{\wedge}$ CNX complexes. <i>Journal of Chemical Physics</i> , 2012, 137, 084314.	3.0	28
56	Competition of hydrogen, halogen, and pnicoen bonds in the complexes of HARF with XH ₂ P (X=F, Cl,) Tj ETQq0 0 0 gBT /Overlock 10 T	3.9	28
57	Modulating the strength of tetrel bonding through beryllium bonding. <i>Journal of Molecular Modeling</i> , 2016, 22, 192.	1.8	28
58	Comparison of hydrogen, halogen, and tetrel bonds in the complexes of HARF with YH ₃ X (X = halogen, Y = C and Si). <i>RSC Advances</i> , 2016, 6, 19136-19143.	3.6	28
59	Comparison of If $\hat{\wedge}$ €Hole Tetrel Bonds between TH ₃ F/F ₂ TO and H ₂ CX (X=O, S, Se). <i>ChemPhysChem</i> , 2019, 20, 627-635.	2.1	28
60	Tuning the Competition between Hydrogen and Tetrel Bonds by a Magnesium Bond. <i>ChemPhysChem</i> , 2020, 21, 212-219.	2.1	28
61	Carbene triel bonds between TrR ₃ (Tr $\hat{\wedge}$ %=â€%B, Al) and Nâ€heterocyclic carbenes. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25867.	2.0	27
62	Influence of Hybridization and Cooperativity on the Properties of Au-Bonding Interaction: Comparison with Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2853-2858.	2.5	26
63	Interplay between the If-tetrel bond and If-halogen bond in PhSiF ₃ â ⁴ -iodopyridineâ ^N -base. <i>RSC Advances</i> , 2017, 7, 21713-21720.	3.6	26
64	Tetrel Bond between 6-OTX ₃ -Fulvene and NH ₃ : Substituents and Aromaticity. <i>Molecules</i> , 2019, 24, 10.	3.8	26
65	A highly selective colorimetric and fluorescent probe for quantitative detection of Cu ²⁺ /Co ²⁺ : The unique ON-OFF-ON fluorimetric detection strategy and applications in living cells/zebrafish. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 228, 117763.	3.9	26
66	A dual-functional fluorescent probe for sequential determination of Cu ²⁺ /S ²⁻ and its applications in biological systems. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 243, 118797.	3.9	26
67	A novel hydrazide Schiff base self-assembled nanoprobe for selective detection of human serum albumin and its applications in renal disease surveillance. <i>Journal of Materials Chemistry B</i> , 2020, 8, 8346-8355.	5.8	26
68	A novel double target fluorescence probe for Al ³⁺ /Mg ²⁺ detection with distinctively different responses and its applications in cell imaging. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 261, 120067.	3.9	26
69	A chromone hydrazide Schiff base fluorescence probe with high selectivity and sensitivity for the detection and discrimination of human serum albumin (HSA) and bovine serum albumin (BSA). <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 422, 113576.	3.9	26
70	The dual role of pnicoen as Lewis acid and base and the unexpected interplay between the pnicoen bond and coordination interaction in H ₃ Nâ ^F H ₂ Xâ ^{MCN} (X = P and As; M = Cu, Ag,) Tj ETQq0 0 0 gBT /Over	3.9	26
71	Synergistic and diminutive effects between triel bond and regium bond: Attractive interactions between If $\hat{\wedge}$ €hole and If $\hat{\wedge}$ €hole. <i>Applied Organometallic Chemistry</i> , 2019, 33, e4806.	3.5	25
72	Theoretical study on the cooperativity of hydrogen bonds in (HNC) ₂ â ^{HF} complexes. <i>Computational and Theoretical Chemistry</i> , 2009, 896, 112-115.	1.5	24

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73	The single-electron hydrogen, lithium, and halogen bonds with HBe, H2B, and H3C radicals as the electron donor: an ab initio study. <i>Structural Chemistry</i> , 2012, 23, 411-416.	2.0	24
74	Competition between hydrogen bonds and halogen bonds in complexes of formamidine and hypohalous acids. <i>Journal of Molecular Modeling</i> , 2013, 19, 4529-4535.	1.8	24
75	A new interaction mechanism of LiNH2 with MgH2: magnesium bond. <i>Journal of Molecular Modeling</i> , 2013, 19, 247-253.	1.8	24
76	Enhancement of Iodine-Hydride Interaction by Substitution and Cooperative Effects in NCX-NCl-HMY Complexes. <i>ChemPhysChem</i> , 2012, 13, 3997-4002.	2.1	23
77	Abnormal synergistic effects between Lewis acid-base interaction and halogen bond in $F_{3B} \cdot NCX \cdot NCM$. <i>Molecular Physics</i> , 2015, 113, 3809-3814.	1.7	23
78	Nonadditivity of methyl group in single-electron hydrogen bond of methyl radical-water complex. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 605-611.	2.0	22
79	Prediction and characterization of HCCH...AuX (X = OH, F, Cl, Br, CH3, CCH, CN, and NC) complexes: A σ -Au-bond. <i>Journal of Chemical Physics</i> , 2011, 135, 074304.	3.0	22
80	The structure, properties, and nature of HArF-HOX (X = F, Cl, Br) complex: An ab initio study and an unusual short hydrogen bond. <i>Journal of Computational Chemistry</i> , 2011, 32, 2432-2440.	3.3	22
81	Comparison for σ -hole and π -hole tetrel-bonded complexes involving cyanoacetaldehyde. <i>Molecular Physics</i> , 2018, 116, 222-230.	1.7	22
82	Competition between dihydrogen bond and beryllium bond in complexes between HBeH and HArF: A huge blue shift of distant HAr stretch. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 90, 135-140.	3.9	21
83	Prominent enhancing effects of substituents on the strength of σ -hole tetrel bond. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25448.	2.0	21
84	The effect of methyl group on the cooperativity between three types of hydrogen bond: $O_i \cdots H_A \cdots O$, $C_i \cdots H_A \cdots O$, and $O_i \cdots H_A \cdots i$. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 558-566.	2.0	20
85	Regulation of coin metal substituents and cooperativity on the strength and nature of tetrel bonds. <i>RSC Advances</i> , 2017, 7, 46321-46328.	3.6	20
86	Comparison of tetrel bonds and halogen bonds in complexes of DMSO with $ZF_3 \cdot X$ (Z = C, Si, Ge, Sn, Pb, Bi, Po, At, Fl, Lv, Ts, Og). <i>Journal of Molecular Modeling</i> , 2019, 25, 19.	3.6	19
87	Comparison of σ -hole and π -hole tetrel bonds in complexes of borazine with $TH_3 \cdot F$ and $F_2 \cdot TO/H_2 \cdot TO$ (T = C, Si, Ge). <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25910.	2.0	19
88	How do organic gold compounds and organic halogen molecules interact? Comparison with hydrogen bonds. <i>RSC Advances</i> , 2015, 5, 12488-12497.	3.6	18
89	Novel pnictogen bonding interactions with silylene as an electron donor: covalency, unusual substituent effects and new mechanisms. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9153-9160.	2.8	18
90	Comparison of hydrogen and halogen bonds between dimethyl sulfoxide and hypohalous acid: competition and cooperativity. <i>Molecular Physics</i> , 2017, 115, 1614-1623.	1.7	17

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91	Synergistic and Diminutive Effects between Regium and Aerogen Bonds. <i>ChemPhysChem</i> , 2020, 21, 2426-2431.	2.1	17
92	Is the Fourier Transform Infrared Free-OH Band of <i>n</i> -Butanol Only from Free OHs? Case Studies on the Binary Systems of the Alcohol with CCl ₄ and CHCl ₃ . <i>Journal of Physical Chemistry A</i> , 2020, 124, 6177-6185.	2.5	17
93	Large blue shift of the H ₂ Ar stretching frequency in hydrogen- and halogen-bonded complexes of HArF with dihalogen molecules. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 77, 506-511.	3.9	16
94	What is the role of defects in single-walled carbon nanotubes for nonlinear optical property?. <i>Journal of Materials Chemistry</i> , 2011, 21, 8905.	6.7	16
95	Influence of the protonation of pyridine nitrogen on pnictogen bonding: competition and cooperativity. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11348-11356.	2.8	16
96	Comparison for σ -hole and π -hole tetrel-bonded complexes involving F ₂ C-CFTF ₃ (T = C, Si, and Ge): Substitution, hybridization, and solvation effects. <i>Journal of Fluorine Chemistry</i> , 2018, 207, 38-44.	1.7	16
97	Comparison between Hydrogen and Halogen Bonds in Complexes of 6 α -OX α -Fulvene with Pnictogen and Chalcogen Electron Donors. <i>ChemPhysChem</i> , 2019, 20, 1978-1984.	2.1	16
98	A new unconventional halogen bond C δ^+ -X δ^- -H δ^+ -M between HCCX (X = Cl and Br) and HMH (M = Be and Tl). <i>Journal of Chemical Physics</i> , 2019, 150, 044308.	3.3	15
99	Competition between σ -hole pnictogen bond and π -hole tetrel bond in complexes of CF ₂ =CFZH ₂ (Z = P, As, and Sb). <i>Molecular Physics</i> , 2019, 117, 251-259.	1.7	15
100	Bioinspired surface with special wettability for liquid transportation and separation. <i>Sustainable Materials and Technologies</i> , 2020, 25, e00175.	3.3	15
101	The π -hole tetrel bond between X_2TO and CO_2 : Substituent effects and its potential adsorptivity for CO_2 . <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26251.	2.0	15
102	Weak σ -Hole Trel Bond between C ₅ H ₅ Tr (Tr=B, Al, Ga) and Haloethyne: Substituent and Cooperativity Effects. <i>ChemPhysChem</i> , 2021, 22, 481-487.	2.1	15
103	Rare gas atomic number dependence of the hyperpolarizability for rare gas inserted fluorohydrides, HRgF (Rg=He, Ar, and Kr). <i>Journal of Chemical Physics</i> , 2009, 131, 044308.	3.0	14
104	Interplay between Metal π - π Interactions and Hydrogen Bonds: Some Unusual Synergetic Effects of Coinage Metals and Substituents. <i>ChemPhysChem</i> , 2013, 14, 3341-3347.	2.1	14
105	Influence of substituents on the nature of metal π - π interaction and its cooperativity with halogen bond. <i>Journal of Chemical Physics</i> , 2015, 143, 054308.	3.0	14
106	Trel π -hydride trel bond between ZX ₃ (Z = B and Al; X = H and Me) and THMe ₃ (T = Tl, Pb, Bi, and Sn). <i>Journal of Chemical Physics</i> , 2019, 150, 044308.	3.5	14
107	Coinage-Metal Bond between [1.1.1]Propellane and M ₂ /MCl/MCH ₃ (M = Cu, Ag, and Au): Cooperativity and Substituents. <i>Molecules</i> , 2019, 24, 2601.	3.8	14
108	Novel 2 α -hydroxynaphthalene α -based fluorescent turn α on sensor for highly sensitive and selective detection of Al ³⁺ and its application in imaging <i>in vitro</i> and <i>in vivo</i> . <i>Applied Organometallic Chemistry</i> , 2020, 34, e5812.	3.5	13

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109	Solvent effect on the role of methyl groups in formation of O ^{δ-} ⋯H-O hydrogen bond in dimethyl ether ^{δ-} methanol complex. <i>Computational and Theoretical Chemistry</i> , 2008, 862, 74-79.	1.5	11
110	Partially covalent nature and substitution non-additivity of Au-bonding in H ₂ O ^{δ-} AuCH ₃ complex. <i>Chemical Physics Letters</i> , 2010, 498, 259-262.	2.6	11
111	Effect of substitution and cooperativity on the Cl ^{δ-} F blue shift in single-electron halogen-bonded H ₃ C ^{δ-} ⋯ClF complex. <i>Molecular Physics</i> , 2010, 108, 2021-2026.	1.7	11
112	Theoretical study on gemylenoid H ₂ GeFBeF. <i>Structural Chemistry</i> , 2012, 23, 867-871.	2.0	11
113	Non-additivity between substitution and cooperative effects in enhancing hydrogen bonds. <i>Journal of Chemical Physics</i> , 2014, 141, 244305.	3.0	11
114	Effect of Magnesium Bond on the Competition Between Hydrogen and Halogen Bonds and the Induction of Proton and Halogen Transfer. <i>ChemPhysChem</i> , 2018, 19, 1456-1464.	2.1	11
115	Coinage metal dimers as the noncovalent interaction acceptors: study of the σ -lump interactions. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21152-21161.	2.8	11
116	Comparison of triel bonds with different chalcogen electron donors: Its dependence on triel donor and methyl substitution. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26046.	2.0	11
117	Modulation engineering of <i>in situ</i> cathodic activation of FeP _x based on W-incorporation for the hydrogen evolution reaction. <i>Nanoscale</i> , 2020, 12, 12364-12373.	5.6	11
118	Xe ^{δ-} chalcogen aerogen bond. Effect of substituents and size of chalcogen atom. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4115-4121.	2.8	11
119	THEORETICAL INVESTIGATION ON THE INSERTION REACTIONS OF THE GEMYLENOID H ₂ GeLiF WITH RH (R = F, OH, NH ₂) (R = F, OH, NH ₂) WITH Cl, S, P, Br, I). <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1350003.	1.5	11
120	Substitution reactions of H ₂ GeFBeF with RH (R = F, OH, NH ₂): A theoretical study. <i>Russian Journal of Physical Chemistry A</i> , 2014, 88, 1097-1102.	0.6	10
121	Competitive interaction between halogen and hydrogen bonds in NH ₂ BrHOX (X = F, Cl, and I) Tj ETO _g 1 1 0.784314 rgB 2.0	2.0	9
122	Interplay between Cation ^{δ-} and Coinage ^{δ-} Metal ^{δ-} Oxygen Interactions: An Ab Initio Study and Cambridge Structural Database Survey. <i>ChemPhysChem</i> , 2015, 16, 1008-1016.	2.1	9
123	Competition between halogen bond and hydrogen bond in complexes of superalkali Li ₃ S and halogenated acetylene XCCH (X = F, Cl, Br, and I). <i>International Journal of Quantum Chemistry</i> , 2015, 2.0 115, 99-105.	2.0	9
124	Dinuclear first-row transition metal ^{δ-} (C ₈ Me ₆) ₂ complexes: metal ^{δ-} metal and metal ^{δ-} ligand bonds determined by the d electron configuration of the metal atom. <i>New Journal of Chemistry</i> , 2016, 40, 1988-1996.	2.8	9
125	Abnormal Tetrel Bonds between Formamidine and TH ₃ F: Substituent Effects. <i>ChemistrySelect</i> , 2018, 3, 2842-2849.	1.5	9
126	Comparison of halide donators based on pi ^{δ-} M (M = Cu, Ag, Au), pi ^{δ-} H and pi ^{δ-} halogen bonds. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	1.4	9

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127	The ability of a tetrel bond to transition a neutral amino acid into a zwitterion. <i>Chemical Physics Letters</i> , 2019, 731, 136584.	2.6	9
128	Influence of cooperativity on the frequency shift of the Ar ν H stretch vibration in HArF complexes. <i>Molecular Physics</i> , 2013, 111, 497-504.	1.7	8
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130	Intramolecular Si \cdots O Tetrel Bonding: Tuning of Substituents and Cooperativity. <i>ChemistrySelect</i> , 2017, 2, 11104-11112.	1.5	8
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133	The structure, properties, and nature of HArF \cdots benzene complex: Redshift and blueshift of Ar ν H stretch frequency and rare gas atomic number dependence of hydrogen bonds. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 84, 68-73.	3.9	7
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142	The prominent enhancing effect and mechanism of the methyl group in the X \cdots A \cdots Y (X=O, S). <i>Journal of Molecular Modeling</i> , 2013, 19, 1311-1318.	1.7	6
143	Is a MH (M = Be and Mg) radical a better electron donor in halogen \cdots hydride interaction?: A theoretical comparison with HMH. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1293-1298.	2.0	6
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166	Nature of MoH ⁻ ⋯I bonds in Cp ₂ Mo(L)H ⁻ ⋯I ⁻ complexes (L=H, CN, PPh ₂ , Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5)	3.5	4
167	Tetrel bonds between PhSiF ₃ /PhTH ₃ (T=Si, Ge, Sn) and H ₃ ZO (Z=O, N), Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	2.0	4
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