

Hui-Li Xu

List of Publications by Year in descending order

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202
papers

5,426
citations

81900

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114465

63
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all docs

203
docs citations

203
times ranked

3069
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	The role of nitro group on the excited-state relaxation mechanism of P-Z base pair. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 267, 120549.	3.9	1
3	Promotion of TH3 (T = Si and Ge) group transfer within a tetrel bond by a cation- π interaction. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1113-1119.	2.8	3
4	Spodium and tetrel bonds involving Zn(II)/Cd(II) and their interplay. <i>Chemical Physics</i> , 2022, 556, 111470.	1.9	6
5	Insight into Spodium- π Bonding Characteristics of the MX ₂ - π (M = Zn, Cd and Hg; X = Cl, Br and I) Complexes-A Theoretical Study. <i>Molecules</i> , 2022, 27, 2885.	3.8	4
6	AIE mechanism of 2-(2-hydroxyphenyl) benzothiazole derivatives: CASPT2 and spin-flip study. <i>Dyes and Pigments</i> , 2022, 204, 110396.	3.7	2
7	Resonance-assisted intramolecular triel bonds. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 15015-15024.	2.8	6
8	Unusual substituent effects in the Tr- π -Te triel bond. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26526.	2.0	6
9	Cooperative effects between triel and halogen bonds in complexes of pyridine derivatives: An opposite effect of the nitrogen oxidation on triel and halogen bonds. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26429.	2.0	6
10	A theoretical study on the excited-state deactivation paths for the A ⁺ 5FU dimer. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16089-16106.	2.8	3
11	Theoretical investigation of the nature of $\pi(B\hat{\pi}B)\hat{\pi}M$ interactions in coinage metal π -diborene complexes. <i>New Journal of Chemistry</i> , 2021, 45, 13380-13388.	2.8	5
12	Weak π -Hole Triel 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
13	Graphitic SiC : A potential anode material for Na-ion battery with extremely high storage capacity. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26608.	2.0	2
14	Diboron Bonds Between BX ₃ (X=H, F, CH ₃) and BYZ ₂ (Y=H, F; Z=CO, N ₂ , CNH). <i>ChemPhysChem</i> , 2021, 22, 1461-1469.	2.1	4
15	Can metal halides be electron donors in π -hole and π -hole tetrel bonds? Cooperativity with an alkaline-earth bond. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26771.	2.0	1
16	Group 12 Carbonates and their Binary Complexes with Nitrogen Bases and FH ₂ Z Molecules (Z=P, As, Sb). <i>TJ ETQq0 0 0 rgBT /Overlock 10 T</i>	2.1	7
17	Enhancement of the Tetrel Bond by the Effects of Substituents, Cooperativity, and Electric Field: Transition from Noncovalent to Covalent Bond. <i>ChemPhysChem</i> , 2021, 22, 2305-2312.	2.1	6
18	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

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19	Noncovalent bond between tetrel ĩ-hole and hydride. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10536-10544.	2.8	2
20	Comparison for Electron Donor Capability of Carbon-Bound Halogens in Tetrel Bonds. <i>ACS Omega</i> , 2021, 6, 29037-29044.	3.5	3
21	Chalcogen Bond Involving Zinc(II)/Cadmium(II) Carbonate and Its Enhancement by Spodium Bond. <i>Molecules</i> , 2021, 26, 6443.	3.8	6
22	Tetrel Bonds between Phenyltrifluorosilane and Dimethyl Sulfoxide: Influence of Basis Sets, Substitution and Competition. <i>Molecules</i> , 2021, 26, 7231.	3.8	4
23	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
24	Regular/abnormal variation in the strength and nature of the halogen bond between H ₂ Te and the dihalogens: Prominent effect of methyl substituents. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5468.	3.5	3
25	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
26	Tuning the Competition between Hydrogen and Tetrel Bonds by a Magnesium Bond. <i>ChemPhysChem</i> , 2020, 21, 212-219.	2.1	28
27	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
28	Interactions in Model Ionic Dyads and Triads Containing Tetrel Atoms. <i>Molecules</i> , 2020, 25, 4197.	3.8	3
29	Novel 2- <i>hydroxynaphthalene</i> -based fluorescent turn-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
30	Highly selective and sensitive chemosensor for Al(III) based on isoquinoline Schiff base. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 243, 118754.	3.9	31
31	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
32	A novel hydrazone 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
33	Synergistic and Diminutive Effects between Regium and Aerogen Bonds. <i>ChemPhysChem</i> , 2020, 21, 2426-2431.	2.1	17
34	Effect of carbon hybridization in C-F bond as an electron donor in triel bonds. <i>Journal of Chemical Physics</i> , 2020, 153, 074304.	3.0	6
35	Reliable Comparison of Pnicogen, Chalcogen, and Halogen Bonds in Complexes of 6-OXF2-Fulvene (X =) Tj ETQq1 1,0.784314 rgBT /Ove	3.6	8
36	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

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37	Bioinspired surface with special wettability for liquid transportation and separation. <i>Sustainable Materials and Technologies</i> , 2020, 25, e00175.	3.3	15
38	Complexes of HArF and AuX (X = F, Cl, Br, I). Comparison of Hâ€¦bonds, halogen bonds, Fâ€¦shared bonds and covalent bonds. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5891.	3.5	6
39	Is the Fourier Transform Infrared Free-OH Band of <i>i</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
40	Xeâ€¦chalcogen aerogen bond. Effect of substituents and size of chalcogen atom. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4115-4121.	2.8	11
41	The ĩ€-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
42	Competition between ĩf-hole pnictogen bond and ĩ€-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
43	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
44	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
45	Systematic study of the substitution effect on the tetrel bond between 1,4-diazabicyclo[2.2.2]octane and TH_3X . <i>RSC Advances</i> , 2019, 9, 18459-18466.	3.6	6
46	Coinage metal dimers as the noncovalent interaction acceptors: study of the ĩf-lump interactions. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21152-21161.	2.8	11
47	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
48	Comparison between Hydrogen and Halogen Bonds in Complexes of 6â€¦OXâ€¦Fulvene with Pnictogen and Chalcogen Electron Donors. <i>ChemPhysChem</i> , 2019, 20, 1978-1984.	2.1	16
49	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
50	Tetrel Bond between 6-OTX3-Fulvene and NH ₃ : Substituents and Aromaticity. <i>Molecules</i> , 2019, 24, 10.	3.8	26
51	Synergistic and diminutive effects between triel bond and regium bond: Attractive interactions between ĩ€-hole and ĩf-hole. <i>Applied Organometallic Chemistry</i> , 2019, 33, e4806.	3.5	25
52	Comparison of ĩf-hole and ĩ€-hole tetrel bonds in complexes of borazine with TH_3F and F_2TO/H_2TO (T = C, Si, Ge). <i>International Journal of Quantum Chemistry</i> , 2019, 20, 119, e25910.	2.0	19
53	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
54	Carbene triel bonds between TrR ₃ (Tr = B, Al) and Nâ€¦heterocyclic carbenes. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25867.	2.0	27

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55	Comparison of σ -hole Tetrel Bonds between $\text{TH}_3/\text{F}_2/\text{TO}$ and H_2/CX ($\text{X}=\text{O}, \text{S}, \text{Se}$). <i>ChemPhysChem</i> , 2019, 20, 627-635.	2.1	28
56	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
57	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
58	Nature of $\text{MoH}\cdots\text{I}$ bonds in $\text{Cp}_2\text{Mo}(\text{L})\text{H}\cdots\text{I}\cdots\text{C}$ Complexes ($\text{L}=\text{H}, \text{CN}, \text{PPh}_2$), <i>Tj ETQq0 0 0 rgBT Applied Organometallic Chemistry</i> , 2018, 32, e4258.	3.5	4
59	Comparison for σ -hole and π -hole tetrel-bonded complexes involving $\text{F}_2\text{C-CFTF}_3$ ($\text{T}=\text{C}, \text{Si}, \text{and Ge}$): Substitution, hybridization, and solvation effects. <i>Journal of Fluorine Chemistry</i> , 2018, 207, 38-44.	1.7	16
60	Abnormal Tetrel Bonds between Formamidine and TH_3/F : Substituent Effects. <i>ChemistrySelect</i> , 2018, 3, 2842-2849.	1.5	9
61	Theoretical assessing on the coordination mode and bonding in heteronuclear group 13 dimetallocene. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25461.	2.0	1
62	Comparison for σ -hole and π -hole tetrel-bonded complexes involving cyanoacetaldehyde. <i>Molecular Physics</i> , 2018, 116, 222-230.	1.7	22
63	The π -Tetrel Bond and its Influence on Hydrogen Bonding and Proton Transfer. <i>ChemPhysChem</i> , 2018, 19, 736-743.	2.1	46
64	Understanding the effects of vicinal carbon substituents and configuration on organofluorine hydrogen-bonding interaction. <i>RSC Advances</i> , 2018, 8, 38980-38986.	3.6	3
65	Comparison of halide donators based on $\text{pi}\cdots\text{M}$ ($\text{M}=\text{Cu}, \text{Ag}, \text{Au}$), $\text{pi}\cdots\text{H}$ and $\text{pi}\cdots\text{halogen}$ bonds. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	1.4	9
66	Carbon Excess C_3N : A Potential Candidate as Li-Ion Battery Material. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 37135-37141.	8.0	44
67	Triel-hydride triel bond between ZX_3 ($\text{Z}=\text{B and Al}; \text{X}=\text{H and Me}$) and THMe_3 ($\text{T}=\text{C, Si, and Ge}$). <i>Tj ETQq1 1 0.784314 rgBT</i>	3.5	14
68	Comparative Strengths of Tetrel, Pnicogen, Chalcogen, and Halogen Bonds and Contributing Factors. <i>Molecules</i> , 2018, 23, 1681.	3.8	69
69	Cooperative effects between π -hole triel and π -hole chalcogen bonds. <i>RSC Advances</i> , 2018, 8, 26580-26588.	3.6	33
70	Tetrel bonds between $\text{PhSiF}_3/\text{PhTH}_3$ ($\text{T}=\text{Si}, \text{Ge}, \text{Sn}$) and H_3/ZO ($\text{Z}=\text{N}$), <i>Tj ETQq1 1 0.784314 rgBT</i>	2.0	4
71	Nonlinear optical properties of aluminum nitride nanotubes doped by excess electron: a first principle study. <i>Journal of Molecular Modeling</i> , 2018, 24, 205.	1.8	7
72	Dual function of the boron center of $\text{BH}(\text{CO})_2/\text{BH}(\text{N}_2)_2$ in halogen- and triel-bonded complexes with hypervalent halogens. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 84, 118-124.	2.4	8

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73	Comparison of tetrel bonds in neutral and protonated complexes of pyridine and furan (T = C, Si, and Ge) with NH ₃ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 5550-5559.	2.8	98
74	Interplay between the σ -tetrel bond and σ -halogen bond in PhSiF ₃ -4-iodopyridine-N-base. <i>RSC Advances</i> , 2017, 7, 21713-21720.	3.6	26
75	Carbene tetrel-bonded complexes. <i>Structural Chemistry</i> , 2017, 28, 823-831.	2.0	47
76	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
77	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
78	The ground and excited-state electronic structures of sandwich compounds Cp ₂ (ME) ₂ contain an (ME) ₂ four-membered ring (Cp = C ₅ H ₅ ; M = Ni, Pd, Pt; E = O, S, Se, Te). <i>New Journal of Chemistry</i> , 2017, 41, 12028-12034.	2.8	3
79	The insertion and H ₂ elimination reactions of H ₂ GeFMgF germynoid with RH (R = Cl, SH, PH ₂). <i>Russian Journal of Physical Chemistry A</i> , 2017, 91, 1660-1668.	0.6	2
80	Comparison of σ -hole and π -hole Tetrel Bonds Formed by Pyrazine and 1,4-dicyanobenzene: The Interplay between Anion- π and Tetrel Bonds. <i>ChemPhysChem</i> , 2017, 18, 2442-2450.	2.1	38
81	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
82	Intramolecular Si...O Tetrel Bonding: Tuning of Substituents and Cooperativity. <i>ChemistrySelect</i> , 2017, 2, 11104-11112.	1.5	8
83	Origin of selenium-gold interaction in F ₂ CSe ⁻ AuY (Y = CN, F, Cl, Br, OH, and CH ₃): Synergistic effects. <i>Journal of Chemical Physics</i> , 2016, 144, 114306.	3.0	7
84	Tetrel bond of pseudohalide anions with XH ₃ F (X = C, Si, Ge, and Sn) and its role in S _N 2 reaction. <i>Journal of Chemical Physics</i> , 2016, 145, 224310.	3.0	68
85	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
86	Novel Zn(II)-thiazolone-based solid fluorescent chemosensors: naked-eye detection for acid/base and toluene. <i>RSC Advances</i> , 2016, 6, 52310-52317.	3.6	3
87	Theoretical prediction on the addition reaction of germynoid H ₂ GeFMgF with ethylene. <i>Journal of Theoretical and Computational Chemistry</i> , 2016, 15, 1650022.	1.8	4
88	Structures of the germynoid H ₂ GeZnCl ₂ and its addition reactions with ethylene. <i>Structural Chemistry</i> , 2016, 27, 1819-1829.	2.0	5
89	Comparison of tetrel bonds and halogen bonds in complexes of DMSO with ZF ₃ X (Z = C, Si, Ge, Sn, Pb, Bi, Sb, As, N, P, As, Sb, Bi, Tl, Pb, Sn, Ge, Si, C) Tj ETQq1 1 0.784314 rrgBT /Overl	3.6	19
90	Modulating the strength of tetrel bonding through beryllium bonding. <i>Journal of Molecular Modeling</i> , 2016, 22, 192.	1.8	28

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91	Dinuclear first-row transition metal ^{II} (C8Me6)2 complexes: metal ^{II} -metal and metal ^{II} -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
92	Theoretical study of the cooperative effects between the triel bond and the pnictogen bond in BF3·A·NCXH2·A·Y (X = P, As, Sb; Y = H2O, NH3) complexes. <i>Journal of Molecular Modeling</i> , 2016, 22, 10.	1.8	29
93	Comparison of hydrogen, halogen, and tetrel bonds in the complexes of HArF with YH3 (X = halogen, Y = C and Si). <i>RSC Advances</i> , 2016, 6, 19136-19143.	3.6	28
94	Tetrel bonds between PySiX3 and some nitrogenated bases: Hybridization, substitution, and cooperativity. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 65, 35-42.	2.4	36
95	The aerogen ^{II} bonds involving ^{II} systems. <i>Chemical Physics Letters</i> , 2016, 651, 50-55.	2.6	33
96	Resveratrol Ameliorates Diabetes-Induced Cardiac Dysfunction Through AT1R-ERK/p38 MAPK Signaling Pathway. <i>Cardiovascular Toxicology</i> , 2016, 16, 130-137.	2.7	57
97	Complicated synergistic effects between metal ^{II} - ^{II} interaction and halogen bonding involving MCCX. <i>RSC Advances</i> , 2015, 5, 105160-105168.	3.6	6
98	Influence of substituents on the nature of metal ^{II} - ^{II} interaction and its cooperativity with halogen bond. <i>Journal of Chemical Physics</i> , 2015, 143, 054308.	3.0	14
99	Theoretical prediction on the insertion reactions of the germolenoid H2GeLiF with GeH3X (X = F, Cl). <i>Tj ETQq1 1 0.784314 rgBT /Over 0.6</i>	0.6	314
100	Monolayer Ti ₂ CO 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
101	Influence of F and Se substitution on the structures, stabilities and nature of the complexes between F ₂ CSe and HOX (X = F, Cl, Br, and I). <i>RSC Advances</i> , 2015, 5, 52667-52675.	3.6	7
102	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
103	The dual role of pnictogen as Lewis acid and base and the unexpected interplay between the pnictogen bond and coordination interaction in H ₃ N ⁺ FH ₂ X ⁻ MCN (X = P and As; M = Cu, Ag). <i>Tj ETQq1 1 0.784314</i>	0.6	314
104	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
105	Interplay between Cation ^{II} and Coinage ^I Metal ^I -Oxygen Interactions: An Ab Initio Study and Cambridge Structural Database Survey. <i>ChemPhysChem</i> , 2015, 16, 1008-1016.	2.1	9
106	Structure and magnetic properties of open-ended silicon carbide nanotubes. <i>RSC Advances</i> , 2015, 5, 52754-52758.	3.6	2
107	Structure of H ₂ GeFMgF and its insertion reactions with RH (R = F, OH, NH ₂). <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550004.	1.8	6
108	Se ^{II} -N Chalcogen Bond and Se ^{II} -X Halogen Bond Involving F ₂ CSe: Influence of Hybridization, Substitution, and Cooperativity. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3518-3527.	2.5	45

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109	Theoretical prediction on H ₂ elimination reactions of H ₂ GeLiF with RH (R = Cl, SH, and PH ₂). Russian Journal of Physical Chemistry A, 2015, 89, 812-817.	0.6	2
110	The band gap modulation of monolayer Ti ₂ CO ₂ by strain. RSC Advances, 2015, 5, 30438-30444.	3.6	82
111	Beryllium decorated armchair BC ₂ N nanoribbons: coexistence of planar tetracoordinate carbon and nitrogen moieties. RSC Advances, 2015, 5, 73945-73950.	3.6	8
112	Abnormal synergistic effects between Lewis acid-base interaction and halogen bond in F ₃ B $\cdot\cdot\cdot$ NCX $\cdot\cdot\cdot$ NCM. Molecular Physics, 2015, 113, 3809-3814.	1.7	23
113	Theoretical study of synergistic effects between anion $\cdot\cdot\cdot$ and metal $\cdot\cdot\cdot$ Lp interactions. RSC Advances, 2015, 5, 76912-76918.	3.6	5
114	Competition between halogen bond and hydrogen bond in complexes of superalkali Li ₃ S and halogenated acetylene XCCH (X = F, Cl, Br, and I). International Journal of Quantum Chemistry, 2015, 20, 115, 99-105.	2.0	9
115	Competition and cooperativity between tetrel bond and chalcogen bond in complexes involving F ₂ CX (X = Se and Te). Chemical Physics Letters, 2015, 620, 7-12.	2.6	103
116	Prediction and characterization of halogen bonds involving formamidine and its derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 138, 195-202.	3.9	5
117	Tetrel-Hydride Interaction between XH ₃ F (X = C, Si, Ge, Sn) and HM (M = Li, Na, BeH, MgH). Journal of Physical Chemistry A, 2015, 119, 2217-2224.	2.5	79
118	Halogen bonds with N-heterocyclic carbenes as halogen acceptors: a partially covalent character. Molecular Physics, 2014, 112, 3024-3032.	1.7	29
119	Non-additivity between substitution and cooperative effects in enhancing hydrogen bonds. Journal of Chemical Physics, 2014, 141, 244305.	3.0	11
120	Cooperative and Diminutive Effects of Pnicogen Bonds and Cation $\cdot\cdot\cdot$ Interactions. ChemPhysChem, 2014, 15, 500-506.	2.1	38
121	A quantum chemical study of the structures, stability, and spectroscopy of halogen- and hydrogen-bonded complexes between cyanoacetaldehyde and hypochlorous acids. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 121, 157-163.	3.9	7
122	Mutual influence between covalent and noncovalent interactions in H ₃ N $\cdot\cdot\cdot$ MCN $\cdot\cdot\cdot$ XF (X = H, F, Cl, Br, I). Journal of Physical Chemistry A, 2014, 118, 10000-10005.	1.7	85
123	Influence of the nature of hydrogen halides and metal cations on the interaction types between borazine and hydrogen halides. Journal of Molecular Modeling, 2014, 20, 2089.	1.8	3
124	Novel non-covalent interactions involved with the Al ₁₃ M cluster (M = Li, Na, K, Cu, Ag). Journal of Physical Chemistry A, 2014, 118, 10000-10005.	1.7	3
125	Interplay between tetrel bonding and hydrogen bonding interactions in complexes involving F ₂ XO (X=C and Si) and HCN. Computational and Theoretical Chemistry, 2014, 1050, 51-57.	2.5	55
126	Is there halogen bonding or lone pair $\cdot\cdot\cdot$ interaction formed between borazine and some halogenated compounds?. Physical Chemistry Chemical Physics, 2014, 16, 159-165.	2.8	30

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127	Hydrogen bonding involved with superhalogen MX ₂ NY: its influence on the structure and stability of the superhalogen. <i>Molecular Physics</i> , 2014, 112, 1947-1953.	1.7	3
128	Novel CX ⁻ halogen bonds in complexes of acetylene and its derivatives of Na and MPH ₃ (M=Cu, Ag, Au) with XCCF (X=Cl, Br, I). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 127, 10-15.	3.9	4
129	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
130	Complexes between hypohalous acids and phosphine derivatives. Pnicogen bond versus halogen bond versus hydrogen bond. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 132, 271-277.	3.9	33
131	A σ -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
132	Is a MH (M = Be and Mg) radical a better electron donor in halogen σ -hydride interaction?: A theoretical comparison with HMH. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1293-1298.	2.0	6
133	Interplay between Metal σ - π Interactions and Hydrogen Bonds: Some Unusual Synergetic Effects of Coinage Metals and Substituents. <i>ChemPhysChem</i> , 2013, 14, 3341-3347.	2.1	14
134	Spin-orbit ab initio investigation of the photodissociation of C ₂ H ₅ Br. <i>Structural Chemistry</i> , 2013, 24, 1591-1595.	2.0	2
135	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
136	A new interaction mechanism of LiNH ₂ with MgH ₂ : magnesium bond. <i>Journal of Molecular Modeling</i> , 2013, 19, 247-253.	1.8	24
137	Effect of superalkali substituents on the strengths and properties of hydrogen and halogen bonds. <i>Journal of Molecular Modeling</i> , 2013, 19, 1311-1318.	1.8	7
138	Competition of hydrogen, halogen, and pnicogen bonds in the complexes of HArF with XH ₂ P (X=F, Cl, Br, I). <i>Journal of Molecular Modeling</i> , 2013, 19, 1319-1328.	3.9	28
139	Influence of cooperativity on the frequency shift of the Ar σ -H stretch vibration in HArF complexes. <i>Molecular Physics</i> , 2013, 111, 497-504.	1.7	8
140	Influence of insertion of a noble gas atom on halogen bonding in H ₂ O σ -XCCNgF and H ₃ N σ -XCCNgF (X=Cl and Br; Ng=Ar, Kr, and Xe) complexes. <i>Structural Chemistry</i> , 2013, 24, 25-31.	2.0	5
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143	Competition between hydrogen bond and σ -hole interaction in SCS-HArF and SeCSe-HArF complexes. <i>Molecular Physics</i> , 2012, 110, 2969-2975.	1.7	2
144	Substitution, cooperative, and solvent effects on σ - pnicogen bonds in the FH ₂ P and FH ₂ As complexes. <i>Journal of Molecular Modeling</i> , 2012, 18, 4325-4332.	1.8	56

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145	Cooperative and substitution effects in enhancing strengths of halogen bonds in FClâ€ˆCNX complexes. <i>Journal of Chemical Physics</i> , 2012, 137, 084314.	3.0	28
146	Structures, properties and nature of DMSOâ€ˆXY (XY=ClF and BrF) complexes: Redshift and blueshift of SO stretch. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 97, 600-605.	3.9	4
147	Competition of chalcogen bond, halogen bond, and hydrogen bond in SCSHOX and SeCSeHOX (X=Cl) Tj ETQq1 1 0.784314 rgBT /Over	2.5	75
148	Mediated effect of substitutes on the strength of both types of hydrogen bonds formed between HNgF (Ng=He, Ar, Kr) and HCCX (X=H, F, Cl, Br, I, At, and CH3). <i>Computational and Theoretical Chemistry</i> , 2012, 992, 150-155.	2.5	4
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150	Prediction and characterization of a chalcogenâ€ˆhydride interaction with metal hybrids as an electron donor in F2CSâ€ˆHM and F2CSeâ€ˆHM (M = Li, Na, BeH, MgH, MgCH3) complexes. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 3025.	2.8	31
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152	Theoretical study on the insertion reactions of the germolenoid H2GeClMgCl with RH (R = F, OH, NH2). <i>Russian Journal of Physical Chemistry A</i> , 2012, 86, 1969-1973.	0.6	7
153	CASPT2 study on low-lying states of HMgO and HOMg. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1209-1214.	2.0	3
154	Theoretical prediction on HAlS+ and HSAI+ cations using multiconfiguration second-order perturbation theory. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2499-2503.	2.0	2
155	Competitive interaction between halogen and hydrogen bonds in NH₂Brâ€ˆHOX (X = F, Cl, and) Tj ETQq1 1 0.784314 rgBT	2.0	9
156	Concerted Interaction between Pnicogen and Halogen Bonds in XClâ€ˆFH₂Piâ€ˆNH₃ (X=F, OH, CN, NC, and FCC). <i>ChemPhysChem</i> , 2012, 13, 1205-1212.	2.1	124
157	Theoretical study on germolenoid H2GeFBeF. <i>Structural Chemistry</i> , 2012, 23, 867-871.	2.0	11
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159	The structure, properties, and nature of Câ€ˆBrâ€ˆF halogen bond involving HARF: Substitution, hybridization, and nonadditivity. <i>Journal of Fluorine Chemistry</i> , 2012, 135, 207-212.	1.7	7
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161	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
162	CASPT2 study on low-lying states of HBS⁺ and HSB⁺ cations. <i>Molecular Physics</i> , 2011, 109, 2671-2677.	1.7	5

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164	Some measures for making halogen bonds stronger than hydrogen bonds in H₂CSâ€“HOX (X) Tj ETQq0 0 0 rgBT /Overlock	2.8	66
165	Influence of Hybridization and Cooperativity on the Properties of Au-Bonding Interaction: Comparison with Hydrogen Bonds. Journal of Physical Chemistry A, 2011, 115, 2853-2858.	2.5	26
166	The prominent enhancing effect and mechanism of the methyl group in the XÂ•Â•Y (X=O, S,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 632 831-838.	1.7	6
167	The structure, properties, and nature of HARFâ€“benzene complex: Redshift and blueshift of Arâ€“H stretch frequency and rare gas atomic number dependence of hydrogen bonds. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 84, 68-73.	3.9	7
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175	Competition between hydrogen bond and halogen bond in complexes of formaldehyde with hypohalous acids. Physical Chemistry Chemical Physics, 2010, 12, 6837.	2.8	92
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179	Assignment on the X, A, B, C, and D states of the C₆H₅Br⁺ cation based on highâ€“level calculations. International Journal of Quantum Chemistry, 2010, 110, 2683-2688.	2.0	2
180	Prominent Effect of Alkali Metals in Halogen-Bonded Complex of MCCBrâ€“NCMâ€“ ² (M and Mâ€“ ² = H, Li, Na, F,) Tj ETQq0 0 0 rgBT /Overlock	2.5	34

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181	Surprising enhancing effect of methyl group on the strength of O \cdots XF and S \cdots XF (X=Cl and Br) halogen bonds. <i>Journal of Chemical Physics</i> , 2010, 133, 114303.	3.0	29
182	Effect of substitution and cooperativity on the Cl \cdots F blue shift in single-electron halogen-bonded H ₃ C \cdots ClF complex. <i>Molecular Physics</i> , 2010, 108, 2021-2026.	1.7	11
183	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
184	Theoretical study on the π -hydrogen-bonded complex between HArF and ethylene. <i>Computational and Theoretical Chemistry</i> , 2009, 897, 69-72.	1.5	3
185	Nonadditivity of methyl group in single-electron hydrogen bond of methyl radical \cdots water complex. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 605-611.	2.0	22
186	Theoretical study on HBC [•] and HCB [•] anions using multiconfiguration second-order perturbation theory. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1074-1079.	2.0	4
187	Theoretical study on the cooperativity of hydrogen bonds in (HNC) ₂ \cdots HF complexes. <i>Computational and Theoretical Chemistry</i> , 2009, 896, 112-115.	1.5	24
188	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
189	Ab Initio Study of Lithium-Bonded Complexes with Carbene as an Electron Donor. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14156-14160.	2.5	43
190	Prediction and characterization of the HMgH \cdots LiX (X = H, OH, F, CCH, CN, and NC) complexes: a lithium \cdots hydride lithium bond. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 2402.	2.8	64
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192	Cooperativity between the Dihydrogen Bond and the N \cdots HC Hydrogen Bond in LiH \cdots (HCN) _n Complexes. <i>ChemPhysChem</i> , 2008, 9, 1942-1946.	2.1	47
193	Cooperativity between the Halogen Bond and the Hydrogen Bond in H ₃ N \cdots XY \cdots HF Complexes (X, Y=F, Cl, Br). <i>ChemPhysChem</i> , 2008, 9, 2265-2269.	2.1	152
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195	Solvent effect on the role of methyl groups in formation of O \cdots HO hydrogen bond in dimethyl ether \cdots methanol complex. <i>Computational and Theoretical Chemistry</i> , 2008, 862, 74-79.	1.5	11
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197	Influence of Substitution, Hybridization, and Solvent on the Properties of C \cdots HO Single-Electron Hydrogen Bond in CH ₃ \cdots H ₂ O Complex. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5258-5263.	2.5	53
198	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

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200	Cooperativity between OHâˆ•âˆ•O and CHâˆ•âˆ•O Hydrogen Bonds Involving Dimethyl Sulfoxideâˆ•H₂Oâˆ•H₂O Complex. Journal of Physical Chemistry A, 2007, 111, 10166-10169.	2.5	81
201	The Role of Methyl Groups in the Formation of Hydrogen Bond in DMSOâˆ•Methanol Mixtures. Journal of the American Chemical Society, 2006, 128, 1438-1439.	13.7	183
202	Comparison of Î€(Bi&3/4B)âˆ•M bond and luminescence behavior of <sc>group 11/12</sc> metal <sc>Î€âˆ•diborene</sc> complexes: Theoretical investigation. International Journal of Quantum Chemistry, 0, , .	2.0	0