Hui-Li Xu

List of Publications by Year in Descending Order

197 papers	4,457 citations	36 h-index	57 g-index
203 ext. papers	4,966 ext. citations	3.2 avg, IF	5.92 L-index

#	Paper	IF	Citations
197	Spodium and tetrel bonds involving Zn(II)/Cd(II) and their interplay. *Chemical Physics*, **2022**, 556, 111470	2.3	1
196	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). *Journal of Photochemistry and Photobiology A: Chemistry*, **2022**, 422, 113576	4.7	3
195	AIE mechanism of 2-(2-hydroxyphenyl) benzothiazole derivatives: CASPT2 and spin-flip study. *Dyes and Pigments*, **2022**, 110396	4.6	
194	The role of nitro group on the excited-state relaxation mechanism of P-Z base pair. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 120549	4.4	
193	Comparison for Electron Donor Capability of Carbon-Bound Halogens in Tetrel Bonds. *ACS Omega*, **2021**, 6, 29037-29044	3.9	1
192	Chalcogen Bond Involving Zinc(II)/Cadmium(II) Carbonate and Its Enhancement by Spodium Bond. *Molecules*, **2021**, 26,	4.8	2
191	Diboron Bonds Between BX (X=H, F, CH) and BYZ (Y=H, F; Z=CO, N , CNH). *ChemPhysChem*, **2021**, 22, 1461-1469	3.2	4
190	Can metal halides be electron donors in hole and hole tetrel bonds? Cooperativity with an alkaline-earth bond. *International Journal of Quantum Chemistry*, **2021**, 121, e26771	2.1	
189	Unusual substituent effects in the TrTe triel bond. *International Journal of Quantum Chemistry*, **2021**, 121, e26526	2.1	3
188	Cooperative effects between triel and halogen bonds in complexes of pyridine derivatives: An opposite effect of the nitrogen oxidation on triel and halogen bonds. *International Journal of Quantum Chemistry*, **2021**, 121, e26429	2.1	2
187	A theoretical study on the excited-state deactivation paths for the A-5FU dimer. *Physical Chemistry Chemical Physics*, **2021**, 23, 16089-16106	3.6	2
186	Theoretical investigation of the nature of (BB)?M interactions in coinage metal diborene complexes. *New Journal of Chemistry*, **2021**, 45, 13380-13388	3.6	1
185	Weak Hole Triel Bond between C H Tr (Tr=B, Al, Ga) and Haloethyne: Substituent and Cooperativity Effects. *ChemPhysChem*, **2021**, 22, 481-487	3.2	7
184	Graphitic SiC: A potential anode material for Na-ion battery with extremely high storage capacity. *International Journal of Quantum Chemistry*, **2021**, 121, e26608	2.1	1
183	Group 12 Carbonates and their Binary Complexes with Nitrogen Bases and FH Z Molecules (Z=P, As, Sb): Synergism in Forming Ternary Complexes. *ChemPhysChem*, **2021**, 22, 1698-1705	3.2	4
182	Enhancement of the Tetrel Bond by the Effects of Substituents, Cooperativity, and Electric Field: Transition from Noncovalent to Covalent Bond. *ChemPhysChem*, **2021**, 22, 2305-2312	3.2	3
181	A novel double target fluorescence probe for Al/Mg detection with distinctively different responses and its applications in cell imaging. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 261, 120067	4.4	7

180	Noncovalent bond between tetrel hole and hydride. *Physical Chemistry Chemical Physics*, **2021**, 23, 10536-10544	3.6	4
179	Reliable Comparison of Pnicogen, Chalcogen, and Halogen Bonds in Complexes of 6-OXF-Fulvene (X = As, Sb, Se, Te, Be, I) With Three Electron Donors. *Frontiers in Chemistry*, **2020**, 8, 608486	5	3
178	Modulation engineering of in situ cathodic activation of FeP based on W-incorporation for the hydrogen evolution reaction. *Nanoscale*, **2020**, 12, 12364-12373	7.7	3
177	Bioinspired surface with special wettability for liquid transportation and separation. *Sustainable Materials and Technologies*, **2020**, 25, e00175	5.3	7
176	Complexes of HArF and AuX (X = F, Cl, Br, I). Comparison of H-bonds, halogen bonds, F-shared bonds and covalent bonds. *Applied Organometallic Chemistry*, **2020**, 34, e5891	3.1	4
175	Is the Fourier Transform Infrared Free-OH Band of -Butanol Only from Free OHs? Case Studies on the Binary Systems of the Alcohol with CCl and CHCl. *Journal of Physical Chemistry A*, **2020**, 124, 6177-6185	2.8	6
174	Xechalcogen aerogen bond. Effect of substituents and size of chalcogen atom. *Physical Chemistry Chemical Physics*, **2020**, 22, 4115-4121	3.6	4
173	The hole tetrel bond between X2TO and CO2: Substituent effects and its potential adsorptivity for CO2. *International Journal of Quantum Chemistry*, **2020**, 120, e26251	2.1	8
172	Regular/abnormal variation in the strength and nature of the halogen bond between H2Te and the dihalogens: Prominent effect of methyl substituents. *Applied Organometallic Chemistry*, **2020**, 34, e5468	3.1	2
171	The development of coumarin Schiff base system applied as highly selective fluorescent/colorimetric probes for Cu2+ and tumor biomarker glutathione detection. *Dyes and Pigments*, **2020**, 175, 108156	4.6	32
170	Tuning the Competition between Hydrogen and Tetrel Bonds by a Magnesium Bond. *ChemPhysChem*, **2020**, 21, 212-219	3.2	24
169	A highly selective colorimetric and fluorescent probe for quantitative detection of Cu/Co: The unique ON-OFF-ON fluorimetric detection strategy and applications in living cells/zebrafish. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 228, 117763	4.4	11
168	Interactions in Model Ionic Dyads and Triads Containing Tetrel Atoms. *Molecules*, **2020**, 25,	4.8	2
167	Novel 2-hydroxynaphthalene-based fluorescent turn-on sensor for highly sensitive and selective detection of Al3+ and its application in imaging in vitro and in vivo. *Applied Organometallic Chemistry*, **2020**, 34, e5812	3.1	5
166	Highly selective and sensitive chemosensor for Al(III) based on isoquinoline Schiff base. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 243, 118754	4.4	15
165	A dual-functional fluorescent probe for sequential determination of Cu/S and its applications in biological systems. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 243, 118797	4.4	12
164	A novel hydrazide Schiff base self-assembled nanoprobe for selective detection of human serum albumin and its applications in renal disease surveillance. *Journal of Materials Chemistry B*, **2020**, 8, 8346-8355	7.3	11
163	Synergistic and Diminutive Effects between Regium and Aerogen Bonds. *ChemPhysChem*, **2020**, 21, 2426-2431	3.2	9

162	Effect of carbon hybridization in C-F bond as an electron donor in triel bonds. *Journal of Chemical Physics*, **2020**, 153, 074304	3.9	4
161	Comparison of triel bonds with different chalcogen electron donors: Its dependence on triel donor and methyl substitution. *International Journal of Quantum Chemistry*, **2020**, 120, e26046	2.1	9
160	Coinage metal dimers as the noncovalent interaction acceptors: study of the lump interactions. *Physical Chemistry Chemical Physics*, **2019**, 21, 21152-21161	3.6	9
159	A bioinspired hybrid membrane with wettability and topology anisotropy for highly efficient fog collection. *Journal of Materials Chemistry A*, **2019**, 7, 124-132	13	66
158	Comparison between Hydrogen and Halogen Bonds in Complexes of 6-OX-Fulvene with Pnicogen and Chalcogen Electron Donors. *ChemPhysChem*, **2019**, 20, 1978-1984	3.2	12
157	A dual functional turn-on non-toxic chemosensor for highly selective and sensitive visual detection of Mg and Zn: the solvent-controlled recognition effect and bio-imaging application. *Analyst, The*, **2019**, 144, 4024-4032	5	36
156	Competition between hole pnicogen bond and hole tetrel bond in complexes of CF2=CFZH2 (Z = P, As, and Sb). *Molecular Physics*, **2019**, 117, 251-259	1.7	14
155	Coinage-Metal Bond between [1.1.1]Propellane and M/MCl/MCH (M = Cu, Ag, and Au): Cooperativity and Substituents. *Molecules*, **2019**, 24,	4.8	9
154	The ability of a tetrel bond to transition a neutral amino acid into a zwitterion. *Chemical Physics Letters*, **2019**, 731, 136584	2.5	7
153	Systematic study of the substitution effect on the tetrel bond between 1,4-diazabicyclo[2.2.2]octane and THX.. *RSC Advances*, **2019**, 9, 18459-18466	3.7	5
152	Synergistic and diminutive effects between triel bond and regium bond: Attractive interactions between hole and hole. *Applied Organometallic Chemistry*, **2019**, 33, e4806	3.1	21
151	Comparison of hole and hole tetrel bonds in complexes of borazine with TH3F and F2TO/H2TO (T = C, Si, Ge). *International Journal of Quantum Chemistry*, **2019**, 119, e25910	2.1	14
150	A high performance 2-hydroxynaphthalene Schiff base fluorescent chemosensor for Al and its applications in imaging of living cells and zebrafish in vivo. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2019**, 207, 31-38	4.4	38
149	Carbene triel bonds between TrR3 (Tr = B, Al) and N-heterocyclic carbenes. *International Journal of Quantum Chemistry*, **2019**, 119, e25867	2.1	24
148	Comparison of /Hole Tetrel Bonds between TH F/F TO and H CX (X=O, S, Se). *ChemPhysChem*, **2019**, 20, 627-635	3.2	18
147	Tetrel Bond between 6-OTX-Fulvene and NH-Substituents and Aromaticity. *Molecules*, **2018**, 24,	4.8	11
146	Effect of Magnesium Bond on the Competition Between Hydrogen and Halogen Bonds and the Induction of Proton and Halogen Transfer. *ChemPhysChem*, **2018**, 19, 1456-1464	3.2	7
145	Highly selective and sensitive turn-on fluorescent sensor for detection of Al based on quinoline-base Schiff base. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2018**, 195, 157-164	4.4	58

144	Nature of MoH□□ bonds in Cp2Mo(L)H□□-C?C-R Complexes (L=H, CN, PPh2, C(CH3)3; R=NO2, Cl, Br, H, OH, CH3, NH2). *Applied Organometallic Chemistry*, **2018**, 32, e4258	3.1	2
143	Comparison for □hole and □hole tetrel-bonded complexes involving F2CCFTF3 (TC, Si, and Ge): Substitution, hybridization, and solvation effects. *Journal of Fluorine Chemistry*, **2018**, 207, 38-44	2.1	16
142	Abnormal Tetrel Bonds between Formamidine and TH3F: Substituent Effects. *ChemistrySelect*, **2018**, 3, 2842-2849	1.8	7
141	Theoretical assessing on the coordination mode and bonding in heteronuclear group-13 dimetallocene. *International Journal of Quantum Chemistry*, **2018**, 118, e25461	2.1	1
140	Comparison for □hole and □hole tetrel-bonded complexes involving cyanoacetaldehyde. *Molecular Physics*, **2018**, 116, 222-230	1.7	20
139	Cooperative effects between □hole triel and □hole chalcogen bonds.. *RSC Advances*, **2018**, 8, 26580-26588	3.7	25
138	Tetrel bonds between PhSiF3/PhTH3 (T = Si, Ge, Sn) and H3ZO (Z = N, P, As): A pentacoordinate silicon (IV) complex. *International Journal of Quantum Chemistry*, **2018**, 118, e25660	2.1	3
137	Nonlinear optical properties of aluminum nitride nanotubes doped by excess electron: a first principle study. *Journal of Molecular Modeling*, **2018**, 24, 205	2	5
136	Dual function of the boron center of BH(CO)/BH(N) in halogen- and triel-bonded complexes with hypervalent halogens. *Journal of Molecular Graphics and Modelling*, **2018**, 84, 118-124	2.8	8
135	The □Tetrel Bond and its Influence on Hydrogen Bonding and Proton Transfer. *ChemPhysChem*, **2018**, 19, 736-743	3.2	39
134	Understanding the effects of vicinal carbon substituents and configuration on organofluorine hydrogen-bonding interaction.. *RSC Advances*, **2018**, 8, 38980-38986	3.7	2
133	Comparison of halide donators based on pi□□M (M = Cu, Ag, Au), pi□□H and pi□□halogen bonds. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	6
132	Carbon Excess CN: A Potential Candidate as Li-Ion Battery Material. *ACS Applied Materials & Interfaces*, **2018**, 10, 37135-37141	9.5	26
131	Triel□ydride triel bond between ZX3 (Z = B and Al; X = H and Me) and THMe3 (T = Si, Ge and Sn). *Applied Organometallic Chemistry*, **2018**, 32, e4367	3.1	13
130	Comparative Strengths of Tetrel, Pnicogen, Chalcogen, and Halogen Bonds and Contributing Factors. *Molecules*, **2018**, 23,	4.8	54
129	Comparison of tetrel bonds in neutral and protonated complexes of pyridineTF and furanTF (T = C, Si, and Ge) with NH. *Physical Chemistry Chemical Physics*, **2017**, 19, 5550-5559	3.6	90
128	Interplay between the □etrel bond and □halogen bond in PhSiF3?4-iodopyridine?N-base. *RSC Advances*, **2017**, 7, 21713-21720	3.7	22
127	Carbene tetrel-bonded complexes. *Structural Chemistry*, **2017**, 28, 823-831	1.8	36

126	Comparison of hydrogen and halogen bonds between dimethyl sulfoxide and hypohalous acid: competition and cooperativity. *Molecular Physics*, **2017**, 115, 1614-1623	1.7	12
125	Regulation of coin metal substituents and cooperativity on the strength and nature of tetrel bonds. *RSC Advances*, **2017**, 7, 46321-46328	3.7	14
124	The ground and excited-state electronic structures of sandwich compounds Cp2(ME)2 contain an (ME)2 four-membered ring (Cp = C5H5; M = Ni, Pd, Pt; E = O, S, Se, Te). *New Journal of Chemistry*, **2017**, 41, 12028-12034	3.6	1
123	The insertion and H2 elimination reactions of H2GeFMgF germylenoid with RH (R = Cl, SH, PH2). *Russian Journal of Physical Chemistry A*, **2017**, 91, 1660-1668	0.7	1
122	Comparison of □-Hole and □-Hole Tetrel Bonds Formed by Pyrazine and 1,4-Dicyanobenzene: The Interplay between Anion-□ and Tetrel Bonds. *ChemPhysChem*, **2017**, 18, 2442-2450	3.2	36
121	Prominent enhancing effects of substituents on the strength of □□□hole tetrel bond. *International Journal of Quantum Chemistry*, **2017**, 117, e25448	2.1	19
120	Intramolecular Si???O Tetrel Bonding: Tuning of Substituents and Cooperativity. *ChemistrySelect*, **2017**, 2, 11104-11112	1.8	6
119	Resveratrol Ameliorates Diabetes-Induced Cardiac Dysfunction Through AT1R-ERK/p38 MAPK Signaling Pathway. *Cardiovascular Toxicology*, **2016**, 16, 130-7	3.4	50
118	Modulating the strength of tetrel bonding through beryllium bonding. *Journal of Molecular Modeling*, **2016**, 22, 192	2	23
117	Dinuclear first-row transition metal(C8Me6)2 complexes: metal□metal and metal□ligand bonds determined by the d electron configuration of the metal atom. *New Journal of Chemistry*, **2016**, 40, 1988-1996	3.6	8
116	Theoretical study of the cooperative effects between the triel bond and the pnicogen bond in BF3□□NCXH2□□Y (X = P, As, Sb; Y = H2O, NH3) complexes. *Journal of Molecular Modeling*, **2016**, 22, 10	2	26
115	Comparison of hydrogen, halogen, and tetrel bonds in the complexes of HArF with YH3X (X = halogen, Y = C and Si). *RSC Advances*, **2016**, 6, 19136-19143	3.7	26
114	Tetrel bonds between PySiX3 and some nitrogenated bases: Hybridization, substitution, and cooperativity. *Journal of Molecular Graphics and Modelling*, **2016**, 65, 35-42	2.8	33
113	The aerogen□bonds involving □systems. *Chemical Physics Letters*, **2016**, 651, 50-55	2.5	29
112	Origin of selenium-gold interaction in F2CSe?AuY (Y = CN, F, Cl, Br, OH, and CH3): Synergistic effects. *Journal of Chemical Physics*, **2016**, 144, 114306	3.9	5
111	Tetrel bond of pseudohalide anions with XHF (X = C, Si, Ge, and Sn) and its role in S2 reaction. *Journal of Chemical Physics*, **2016**, 145, 224310	3.9	60
110	Influence of the protonation of pyridine nitrogen on pnicogen bonding: competition and cooperativity. *Physical Chemistry Chemical Physics*, **2016**, 18, 11348-56	3.6	14
109	Novel Zn(II)-thiazolone-based solid fluorescent chemosensors: naked-eye detection for acid/base and toluene. *RSC Advances*, **2016**, 6, 52310-52317	3.7	2

108	Theoretical prediction on the addition reaction of germylenoid H2GeFMgF with ethylene. *Journal of Theoretical and Computational Chemistry*, **2016**, 15, 1650022	1.8	3
107	Structures of the germylenoid H2GeZnCl2 and its addition reactions with ethylene. *Structural Chemistry*, **2016**, 27, 1819-1829	1.8	4
106	Comparison of tetrel bonds and halogen bonds in complexes of DMSO with ZF3X (Z = C and Si; X = halogen). *RSC Advances*, **2016**, 6, 79245-79253	3.7	18
105	The dual role of pnicogen as Lewis acid and base and the unexpected interplay between the pnicogen bond and coordination interaction in H3N?FH2X?MCN (X = P and As; M = Cu, Ag, and Au). *New Journal of Chemistry*, **2015**, 39, 2067-2074	3.6	24
104	Novel pnicogen bonding interactions with silylene as an electron donor: covalency, unusual substituent effects and new mechanisms. *Physical Chemistry Chemical Physics*, **2015**, 17, 9153-60	3.6	18
103	Interplay between cation-π and coinage-metal-oxygen interactions: an ab initio study and Cambridge Structural Database survey. *ChemPhysChem*, **2015**, 16, 1008-16	3.2	8
102	Structure and magnetic properties of open-ended silicon carbide nanotubes. *RSC Advances*, **2015**, 5, 52754-52758	3.7	5
101	Structure ofH2GeFMgFand its insertion reactions withRH(R=F,OH,NH2). *Journal of Theoretical and Computational Chemistry*, **2015**, 14, 1550004	1.8	5
100	Se⋯N chalcogen bond and Se⋯X halogen bond involving F2C?Se: influence of hybridization, substitution, and cooperativity. *Journal of Physical Chemistry A*, **2015**, 119, 3518-27	2.8	41
99	Theoretical prediction on H2 elimination reactions of H2GeLiF with RH (R = Cl, SH, and PH2). *Russian Journal of Physical Chemistry A*, **2015**, 89, 812-817	0.7	1
98	The band gap modulation of monolayer Ti2CO2 by strain. *RSC Advances*, **2015**, 5, 30438-30444	3.7	52
97	Beryllium decorated armchair BC2N nanoribbons: coexistence of planar tetracoordinate carbon and nitrogen moieties. *RSC Advances*, **2015**, 5, 73945-73950	3.7	6
96	Abnormal synergistic effects between Lewis acid–base interaction and halogen bond in F3B⋯NCX⋯NCM. *Molecular Physics*, **2015**, 113, 3809-3814	1.7	22
95	Theoretical study of synergistic effects between anion-π and metallo-π interactions. *RSC Advances*, **2015**, 5, 76912-76918	3.7	5
94	Competition between halogen bond and hydrogen bond in complexes of superalkali Li3S and halogenated acetylene XCCH (X = F, Cl, Br, and I). *International Journal of Quantum Chemistry*, **2015**, 115, 99-105	2.1	9
93	Competition and cooperativity between tetrel bond and chalcogen bond in complexes involving F2CX (X = Se and Te). *Chemical Physics Letters*, **2015**, 620, 7-12	2.5	95
92	Prediction and characterization of halogen bonds involving formamidine and its derivatives. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 138, 195-202	4.4	5
91	Tetrel-hydride interaction between XH⋯ (X = C, Si, Ge, Sn) and HM (M = Li, Na, BeH, MgH). *Journal of Physical Chemistry A*, **2015**, 119, 2217-24	2.8	73

90	Complicated synergistic effects between metal□interaction and halogen bonding involving MCCX. *RSC Advances*, **2015**, 5, 105160-105168	3.7	6
89	Influence of substituents on the nature of metal?□interaction and its cooperativity with halogen bond. *Journal of Chemical Physics*, **2015**, 143, 054308	3.9	11
88	Theoretical prediction on the insertion reactions of the germylenoid H2GeLiF with GeH3X (X = F, Cl, Br). *Russian Journal of Physical Chemistry A*, **2015**, 89, 1872-1877	0.7	2
87	Monolayer Ti□O□A Promising Candidate for NH□Sensor or Capturer with High Sensitivity and Selectivity. *ACS Applied Materials & Interfaces*, **2015**, 7, 13707-13	9.5	367
86	Influence of F and Se substitution on the structures, stabilities and nature of the complexes between F2CSe and HOX (X = F, Cl, Br, and I). *RSC Advances*, **2015**, 5, 52667-52675	3.7	6
85	How do organic gold compounds and organic halogen molecules interact? Comparison with hydrogen bonds. *RSC Advances*, **2015**, 5, 12488-12497	3.7	17
84	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	2	3
83	Novel non-covalent interactions involved with the Al13M cluster (M = Li, Na, K, Cu, Ag, Au). *Molecular Physics*, **2014**, 112, 2954-2962	1.7	3
82	Interplay between tetrel bonding and hydrogen bonding interactions in complexes involving F2XO (X=C and Si) and HCN. *Computational and Theoretical Chemistry*, **2014**, 1050, 51-57	2	48
81	Is □halogen bonding or lone pair□□□interaction formed between borazine and some halogenated compounds?. *Physical Chemistry Chemical Physics*, **2014**, 16, 159-65	3.6	27
80	Hydrogen bonding involved with superhalogen MX2NY: its influence on the structure and stability of the superhalogen. *Molecular Physics*, **2014**, 112, 1947-1953	1.7	3
79	Novel CX?□halogen bonds in complexes of acetylene and its derivatives of Na and MPH3 (M=Cu, Ag, Au) with XCCF (X=Cl, Br, I). *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 127, 10-5	4.4	4
78	Substitution reactions of H2GeFBeF with RH (R = F, OH, NH2): A theoretical study. *Russian Journal of Physical Chemistry A*, **2014**, 88, 1097-1102	0.7	9
77	Complexes between hypohalous acids and phosphine derivatives. Pnicogen bond versus halogen bond versus hydrogen bond. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 132, 271-7	4.4	30
76	A □hole interaction with radical species as electron donors: does single-electron tetrel bonding exist?. *Physical Chemistry Chemical Physics*, **2014**, 16, 11617-25	3.6	104
75	Halogen bonds with N-heterocyclic carbenes as halogen acceptors: a partially covalent character. *Molecular Physics*, **2014**, 112, 3024-3032	1.7	27
74	Non-additivity between substitution and cooperative effects in enhancing hydrogen bonds. *Journal of Chemical Physics*, **2014**, 141, 244305	3.9	10
73	Cooperative and diminutive effects of pnicogen bonds and cation-□interactions. *ChemPhysChem*, **2014**, 15, 500-6	3.2	34

72	A quantum chemical study of the structures, stability, and spectroscopy of halogen- and hydrogen-boned complexes between cyanoacetaldehyde and hypochlorous acids. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 121, 157-63	4.4	3
71	Mutual influence between covalent and noncovalent interactions in H3NMCNXF (X = H, Li, Cl, Br; M = Ag, Cu, Au). *Molecular Physics*, **2014**, 112, 1081-1088	1.7	3
70	Is a MH (M = Be and Mg) radical a better electron donor in halogen-hydride interaction?: A theoretical comparison with HMH. *International Journal of Quantum Chemistry*, **2013**, 113, 1293-1298	2.1	6
69	Interplay between metal???Interactions and hydrogen bonds: some unusual synergetic effects of coinage metals and substituents. *ChemPhysChem*, **2013**, 14, 3341-7	3.2	13
68	Spin-orbit ab initio investigation of the photodissociation of C2H5Br. *Structural Chemistry*, **2013**, 24, 1591-8595	1.8	2
67	Competition between hydrogen bonds and halogen bonds in complexes of formamidine and hypohalous acids. *Journal of Molecular Modeling*, **2013**, 19, 4529-35	2	20
66	A new interaction mechanism of LiNH2 with MgH2: magnesium bond. *Journal of Molecular Modeling* , **2013**, 19, 247-53	2	18
65	Effect of superalkali substituents on the strengths and properties of hydrogen and halogen bonds. *Journal of Molecular Modeling*, **2013**, 19, 1311-8	2	6
64	Competition of hydrogen, halogen, and pnicogen bonds in the complexes of HArF with XH2P (X=F, Cl, and Br). *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 101, 172-7	4.4	28
63	Influence of cooperativity on the frequency shift of the ArH stretch vibration in HArF complexes. *Molecular Physics*, **2013**, 111, 497-504	1.7	7
62	Influence of insertion of a noble gas atom on halogen bonding in H2OXCCNgF and H3NXCCNgF (X = Cl and Br; Ng = Ar, Kr, and Xe) complexes. *Structural Chemistry*, **2013**, 24, 25-31	1.8	5
61	THEORETICAL INVESTIGATION ON THE INSERTION REACTIONS OF THE GERMYLENOIDH2GeLiFWITHRH(R=Cl,SH,PH2). *Journal of Theoretical and Computational Chemistry*, **2013**, 12, 1350003	1.8	8
60	Competition between dihydrogen bond and beryllium bond in complexes between HBeH and HArF: a huge blue shift of distant H-Ar stretch. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 90, 135-40	4.4	20
59	The structure, properties, and nature of CBr?F halogen bond involving HArF: Substitution, hybridization, and nonadditivity. *Journal of Fluorine Chemistry*, **2012**, 135, 207-212	2.1	7
58	The single-electron hydrogen, lithium, and halogen bonds with HBe, H2B, and H3C radicals as the electron donor: an ab initio study. *Structural Chemistry*, **2012**, 23, 411-416	1.8	22
57	Competition between hydrogen bond and hole interaction in SCS-HArF and SeCSe-HArF complexes. *Molecular Physics*, **2012**, 110, 2969-2975	1.7	2
56	Substitution, cooperative, and solvent effects on pnicogen bonds in the FH(2)P and FH(2)As complexes. *Journal of Molecular Modeling*, **2012**, 18, 4325-32	2	54
55	Cooperative and substitution effects in enhancing strengths of halogen bonds in FClCNX complexes. *Journal of Chemical Physics*, **2012**, 137, 084314	3.9	27

54	Structures, properties and nature of DMSO-XY (XY=ClF and BrF) complexes: redshift and blueshift of S=O stretch. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 97, 600-5	4.4	4
53	Competition of chalcogen bond, halogen bond, and hydrogen bond in SCSHOX and SeCSeHOX (X=Cl and Br) complexes. *Computational and Theoretical Chemistry*, **2012**, 980, 56-61	2	66
52	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). *Computational and Theoretical Chemistry*, **2012**, 992, 150-155	2	4
51	Enhancement of iodine-hydride interaction by substitution and cooperative effects in NCX-NCI-HMY complexes. *ChemPhysChem*, **2012**, 13, 3997-4002	3.2	23
50	Prediction and characterization of a chalcogen-hydride interaction with metal hybrids as an electron donor in F2CS-HM and F2CSe-HM (M = Li, Na, BeH, MgH, MgCH3) complexes. *Physical Chemistry Chemical Physics*, **2012**, 14, 3025-30	3.6	31
49	Pnicogen-hydride interaction between FH2X (X = P and As) and HM (M = ZnH, BeH, MgH, Li, and Na). *Journal of Physical Chemistry A*, **2012**, 116, 2547-53	2.8	73
48	Theoretical study on the insertion reactions of the germylenoid H2GeClMgCl with RH (R = F, OH, NH2). *Russian Journal of Physical Chemistry A*, **2012**, 86, 1969-1973	0.7	6
47	CASPT2 study on low-lying states of HMgO and HOMg. *International Journal of Quantum Chemistry*, **2012**, 112, 1209-1214	2.1	2
46	Theoretical prediction on HAlS+ and HSAl+ cations using multiconfiguration second-order perturbation theory. *International Journal of Quantum Chemistry*, **2012**, 112, 2499-2503	2.1	2
45	Competitive interaction between halogen and hydrogen bonds in NH2Br-HOX (X = F, Cl, and Br) complex. *International Journal of Quantum Chemistry*, **2012**, 112, 2429-2434	2.1	9
44	Concerted interaction between pnicogen and halogen bonds in XCl-FH2P-NH3 (X=F, OH, CN, NC, and FCC). *ChemPhysChem*, **2012**, 13, 1205-12	3.2	117
43	Theoretical study on germylenoid H2GeFBeF. *Structural Chemistry*, **2012**, 23, 867-871	1.8	11
42	THEORETICAL STUDY ON HBeP- AND HPBe- ANIONS USING MULTICONFIGURATION SECOND-ORDER PERTURBATION THEORY. *Journal of Theoretical and Computational Chemistry*, **2012**, 11, 1281-1288	1.8	
41	Prediction and characterization of HCCH⋯AuX (X = OH, F, Cl, Br, CH3, CCH, CN, and NC) complexes: a π-Au-bond. *Journal of Chemical Physics*, **2011**, 135, 074304	3.9	19
40	Some measures for making halogen bonds stronger than hydrogen bonds in H2CS-HOX (X = F, Cl, and Br) complexes. *Physical Chemistry Chemical Physics*, **2011**, 13, 2266-71	3.6	59
39	Influence of hybridization and cooperativity on the properties of Au-bonding interaction: comparison with hydrogen bonds. *Journal of Physical Chemistry A*, **2011**, 115, 2853-8	2.8	24
38	The prominent enhancing effect and mechanism of the methyl group in the X⋯Y (X=O, S, H3CO, H3CS, (H3C)2O, (H3C)2S; Y=HCN, HNC) hydrogen-bonded complex. *Molecular Physics*, **2011**, 109, 831-838	1.7	6
37	The structure, properties, and nature of HArF-benzene complex: redshift and blueshift of Ar-H stretch frequency and rare gas atomic number dependence of hydrogen bonds. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 84, 68-73	4.4	6

36	CASPT2 study on low-lying states of HBN and HNB radicals. *International Journal of Quantum Chemistry*, **2011**, 111, 123-129	2.1	3
35	Theoretical study on low-lying states of HAlO+ and HOAl+ cations. *International Journal of Quantum Chemistry*, **2011**, 111, 4373-4377	2.1	2
34	The prominent enhancing effect of the cation-π interaction on the halogen-hydride halogen bond in M1???C6H5X???HM2. *ChemPhysChem*, **2011**, 12, 2289-95	3.2	41
33	The structure, properties, and nature of HArF-HOX (X = F, Cl, Br) complex: an ab initio study and an unusual short hydrogen bond. *Journal of Computational Chemistry*, **2011**, 32, 2432-40	3.5	21
32	Interplay between halogen bond and lithium bond in MCN-LiCN-XCCH (M = H, Li, and Na; X = Cl, Br, and I) complex: the enhancement of halogen bond by a lithium bond. *Journal of Computational Chemistry*, **2011**, 32, 3296-303	3.5	58
31	What is the role of defects in single-walled carbon nanotubes for nonlinear optical property?. *Journal of Materials Chemistry*, **2011**, 21, 8905		13
30	CASPT2 study on low-lying states of HBS+ and HSB+ cations. *Molecular Physics*, **2011**, 109, 2671-2677	1.7	5
29	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	29
28	Prominent effect of alkali metals in halogen-bonded complex of MCCBr⋯NCM? (M and M? = H, Li, Na, F, NH2, and CH3). *Journal of Physical Chemistry A*, **2010**, 114, 10320-5	2.8	32
27	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	3.9	28
26	Effect of substitution and cooperativity on the Cl⋯F blue shift in single-electron halogen-bonded H3C⋯ClF complex. *Molecular Physics*, **2010**, 108, 2021-2026	1.7	10
25	A new unconventional halogen bond C-X...H-M between HCCX (X = Cl and Br) and HMH (M = Be and Mg): an ab initio study. *Journal of Computational Chemistry*, **2010**, 31, 1662-9	3.5	13
24	Competition between hydrogen bond and halogen bond in complexes of formaldehyde with hypohalous acids. *Physical Chemistry Chemical Physics*, **2010**, 12, 6837-43	3.6	84
23	Ab initio study of the cooperativity between NH⋯N and NH⋯C hydrogen bonds in H3N⋯HNC⋯HNC complex. *Theoretical Chemistry Accounts*, **2010**, 127, 303-309	1.9	30
22	Large blue shift of the H-Ar stretching frequency in hydrogen- and halogen-bonded complexes of HArF with dihalogen molecules. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2010**, 77, 506-11	4.4	16
21	Partially covalent nature and substitution non-additivity of Au-bonding in H2O⋯AuCH3 complex. *Chemical Physics Letters*, **2010**, 498, 259-262	2.5	11
20	Assignment on the X, A, B, C, and D states of the C6H5Br+ cation based on high-level calculations. *International Journal of Quantum Chemistry*, **2010**, 110, 2683-2688	2.1	2
19	Rare gas atomic number dependence of the hyperpolarizability for rare gas inserted fluorohydrides, HRgF (Rg = He, Ar, and Kr). *Journal of Chemical Physics*, **2009**, 131, 044308	3.9	14

18	Theoretical study on the hydrogen-bonded complex between HArF and ethylene. *Computational and Theoretical Chemistry*, **2009**, 897, 69-72		3
17	Nonadditivity of methyl group in single-electron hydrogen bond of methyl radical-water complex. *International Journal of Quantum Chemistry*, **2009**, 109, 605-611	2.1	22
16	Theoretical study on HBC and HCB anions using multiconfiguration second-order perturbation theory. *International Journal of Quantum Chemistry*, **2009**, 109, 1074-1079	2.1	4
15	Theoretical study on the cooperativity of hydrogen bonds in (HNC)2?HF complexes. *Computational and Theoretical Chemistry*, **2009**, 896, 112-115		22
14	An unconventional halogen bond with carbene as an electron donor: An ab initio study. *Chemical Physics Letters*, **2009**, 469, 48-51	2.5	51
13	Ab initio study of lithium-bonded complexes with carbene as an electron donor. *Journal of Physical Chemistry A*, **2009**, 113, 14156-60	2.8	37
12	Prediction and characterization of the HMgHLiX (X = H, OH, F, CCH, CN, and NC) complexes: a lithium-hydride lithium bond. *Physical Chemistry Chemical Physics*, **2009**, 11, 2402-7	3.6	60
11	Regulating function of methyl group in strength of CH...O hydrogen bond: a high-level ab initio study. *Journal of Physical Chemistry A*, **2008**, 112, 3985-90	2.8	44
10	Influence of substitution, hybridization, and solvent on the properties of C-HO single-electron hydrogen bond in CH3-H2O complex. *Journal of Physical Chemistry A*, **2008**, 112, 5258-63	2.8	51
9	Excess infrared absorption spectroscopy and its applications in the studies of hydrogen bonds in alcohol-containing binary mixtures. *Applied Spectroscopy*, **2008**, 62, 166-70	3.1	85
8	Cooperativity between two types of hydrogen bond in H(3)C-HCN-HCN and H(3)C-HNC-HNC complexes. *Journal of Chemical Physics*, **2008**, 128, 154102	3.9	56
7	The effect of methyl group on the cooperativity between three types of hydrogen bond: O?H O, C?H O, and O?H *International Journal of Quantum Chemistry*, **2008**, 108, 558-566	2.1	20
6	Cooperativity between the dihydrogen bond and the NHC hydrogen bond in LiH-(HCN)n Complexes. *ChemPhysChem*, **2008**, 9, 1942-6	3.2	47
5	Cooperativity between the halogen bond and the hydrogen bond in H3N...XY...HF complexes (X, Y=F, Cl, Br). *ChemPhysChem*, **2008**, 9, 2265-9	3.2	145
4	Spectroscopic and theoretical evidence for the cooperativity between red-shift hydrogen bond and blue-shift hydrogen bond in DMSO aqueous solutions. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2008**, 69, 211-5	4.4	42
3	Solvent effect on the role of methyl groups in formation of O HO hydrogen bond in dimethyl ether ethanol complex. *Computational and Theoretical Chemistry*, **2008**, 862, 74-79		10
2	Cooperativity between OH...O and CH...O hydrogen bonds involving dimethyl sulfoxide-H2O-H2O complex. *Journal of Physical Chemistry A*, **2007**, 111, 10166-9	2.8	75
1	The role of methyl groups in the formation of hydrogen bond in DMSO-methanol mixtures. *Journal of the American Chemical Society*, **2006**, 128, 1438-9	16.4	151