

Hui-Li Xu

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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	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, 13707-13	9.5	367
196	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, 1438-9	16.4	151
195	Cooperativity between the halogen bond and the hydrogen bond in H ₃ N...XY...HF complexes (X, Y=F, Cl, Br). <i>ChemPhysChem</i> , 2008 , 9, 2265-9	3.2	145
194	Concerted interaction between pnictogen and halogen bonds in XCl-FH ₂ P-NH ₃ (X=F, OH, CN, NC, and FCC). <i>ChemPhysChem</i> , 2012 , 13, 1205-12	3.2	117
193	A Hole interaction with radical species as electron donors: does single-electron tetrel bonding exist?. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 11617-25	3.6	104
192	Competition and cooperativity between tetrel bond and chalcogen bond in complexes involving F ₂ CX (X = Se and Te). <i>Chemical Physics Letters</i> , 2015 , 620, 7-12	2.5	95
191	Comparison of tetrel bonds in neutral and protonated complexes of pyridineTF and furanTF (T = C, Si, and Ge) with NH ₃ . <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 5550-5559	3.6	90
190	Excess infrared absorption spectroscopy and its applications in the studies of hydrogen bonds in alcohol-containing binary mixtures. <i>Applied Spectroscopy</i> , 2008 , 62, 166-70	3.1	85
189	Competition between hydrogen bond and halogen bond in complexes of formaldehyde with hypohalous acids. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 6837-43	3.6	84
188	Cooperativity between OH...O and CH...O hydrogen bonds involving dimethyl sulfoxide-H ₂ O-H ₂ O complex. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 10166-9	2.8	75
187	Tetrel-hydride interaction between XHB (X = C, Si, Ge, Sn) and HM (M = Li, Na, BeH, MgH). <i>Journal of Physical Chemistry A</i> , 2015 , 119, 2217-24	2.8	73
186	Pnictogen-hydride interaction between FH ₂ X (X = P and As) and HM (M = ZnH, BeH, MgH, Li, and Na). <i>Journal of Physical Chemistry A</i> , 2012 , 116, 2547-53	2.8	73
185	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	13	66
184	Competition of chalcogen bond, halogen bond, and hydrogen bond in SCSHOX and SeCSeHOX (X=Cl and Br) complexes. <i>Computational and Theoretical Chemistry</i> , 2012 , 980, 56-61	2	66
183	Prediction and characterization of the HMgHLiX (X = H, OH, F, CCH, CN, and NC) complexes: a lithium-hydride lithium bond. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 2402-7	3.6	60
182	Tetrel bond of pseudohalide anions with XHF (X = C, Si, Ge, and Sn) and its role in S ₂ reaction. <i>Journal of Chemical Physics</i> , 2016 , 145, 224310	3.9	60
181	Some measures for making halogen bonds stronger than hydrogen bonds in H ₂ CS-HOX (X = F, Cl, and Br) complexes. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 2266-71	3.6	59

180	Highly selective and sensitive turn-on fluorescent sensor for detection of Al based on quinoline-base Schiff base. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018 , 195, 157-164	4.4	58
179	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. <i>Journal of Computational Chemistry</i> , 2011 , 32, 3296-303	3.5	58
178	Cooperativity between two types of hydrogen bond in H(3)C-HCN-HCN and H(3)C-HNC-HNC complexes. <i>Journal of Chemical Physics</i> , 2008 , 128, 154102	3.9	56
177	Substitution, cooperative, and solvent effects on Pnictogen bonds in the FH(2)P and FH(2)As complexes. <i>Journal of Molecular Modeling</i> , 2012 , 18, 4325-32	2	54
176	Comparative Strengths of Tetrel, Pnictogen, Chalcogen, and Halogen Bonds and Contributing Factors. <i>Molecules</i> , 2018 , 23,	4.8	54
175	The band gap modulation of monolayer Ti2CO2 by strain. <i>RSC Advances</i> , 2015 , 5, 30438-30444	3.7	52
174	An unconventional halogen bond with carbene as an electron donor: An ab initio study. <i>Chemical Physics Letters</i> , 2009 , 469, 48-51	2.5	51
173	Influence of substitution, hybridization, and solvent on the properties of C-HO single-electron hydrogen bond in CH3-H2O complex. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 5258-63	2.8	51
172	Resveratrol Ameliorates Diabetes-Induced Cardiac Dysfunction Through AT1R-ERK/p38 MAPK Signaling Pathway. <i>Cardiovascular Toxicology</i> , 2016 , 16, 130-7	3.4	50
171	Interplay between tetrel bonding and hydrogen bonding interactions in complexes involving F2XO (X=C and Si) and HCN. <i>Computational and Theoretical Chemistry</i> , 2014 , 1050, 51-57	2	48
170	Cooperativity between the dihydrogen bond and the NHC hydrogen bond in LiH-(HCN) _n Complexes. <i>ChemPhysChem</i> , 2008 , 9, 1942-6	3.2	47
169	Regulating function of methyl group in strength of CH...O hydrogen bond: a high-level ab initio study. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 3985-90	2.8	44
168	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, 211-5	4.4	42
167	Se...N chalcogen bond and Se...X halogen bond involving F2C?Se: influence of hybridization, substitution, and cooperativity. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 3518-27	2.8	41
166	The prominent enhancing effect of the cation-π interaction on the halogen-hydride halogen bond in M1???C6H5X???HM2. <i>ChemPhysChem</i> , 2011 , 12, 2289-95	3.2	41
165	The π-Tetrel Bond and its Influence on Hydrogen Bonding and Proton Transfer. <i>ChemPhysChem</i> , 2018 , 19, 736-743	3.2	39
164	A high performance 2-hydroxynaphthalene Schiff base fluorescent chemosensor for Al 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	4.4	38
163	Ab initio study of lithium-bonded complexes with carbene as an electron donor. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 14156-60	2.8	37

162	Carbene tetrel-bonded complexes. <i>Structural Chemistry</i> , 2017 , 28, 823-831	1.8	36
161	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. <i>Analyst, The</i> , 2019 , 144, 4024-4032	5	36
160	Comparison of π -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	3.2	36
159	Cooperative and diminutive effects of pnictogen bonds and cation- π interactions. <i>ChemPhysChem</i> , 2014 , 15, 500-6	3.2	34
158	Tetrel bonds between PySiX_3 and some nitrogenated bases: Hybridization, substitution, and cooperativity. <i>Journal of Molecular Graphics and Modelling</i> , 2016 , 65, 35-42	2.8	33
157	Prominent effect of alkali metals in halogen-bonded complex of $\text{MCCBr}_n\text{CM}^?$ (M and $M^? = \text{H, Li, Na, F, NH}_2$, and CH_3). <i>Journal of Physical Chemistry A</i> , 2010 , 114, 10320-5	2.8	32
156	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	4.6	32
155	Prediction and characterization of a chalcogen-hydride interaction with metal hybrids as an electron donor in $\text{F}_2\text{CS-HM}$ and $\text{F}_2\text{CSe-HM}$ (M = Li, Na, BeH, MgH, MgCH_3) complexes. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 3025-30	3.6	31
154	Complexes between hypohalous acids and phosphine derivatives. Pnictogen bond versus halogen bond versus hydrogen bond. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 132, 271-7	4.4	30
153	Ab initio study of the cooperativity between $\text{NH}\cdots\text{N}$ and $\text{NH}\cdots\text{C}$ hydrogen bonds in $\text{H}_3\text{N}\cdots\text{N}\cdots\text{C}\cdots\text{N}$ complex. <i>Theoretical Chemistry Accounts</i> , 2010 , 127, 303-309	1.9	30
152	The aerogen- π bonds involving π systems. <i>Chemical Physics Letters</i> , 2016 , 651, 50-55	2.5	29
151	Competition and cooperativity between hydrogen bond and halogen bond in $\text{HNC}^?(\text{HOBr})_n$ and $(\text{HNC})_n^?\text{HOBr}$ ($n=1$ and 2) systems. <i>Computational and Theoretical Chemistry</i> , 2011 , 963, 417-421	2	29
150	Competition of hydrogen, halogen, and pnictogen bonds in the complexes of HArF with XH_2P ($\text{X}=\text{F, Cl, and Br}$). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 101, 172-7	4.4	28
149	Surprising enhancing effect of methyl group on the strength of $\text{O}^?\text{XF}$ and $\text{S}^?\text{XF}$ ($\text{X}=\text{Cl and Br}$) halogen bonds. <i>Journal of Chemical Physics</i> , 2010 , 133, 114303	3.9	28
148	Is π halogen bonding or lone pair- π interaction formed between borazine and some halogenated compounds?. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 159-65	3.6	27
147	Halogen bonds with N-heterocyclic carbenes as halogen acceptors: a partially covalent character. <i>Molecular Physics</i> , 2014 , 112, 3024-3032	1.7	27
146	Cooperative and substitution effects in enhancing strengths of halogen bonds in $\text{FCl}\cdots\text{CNX}$ complexes. <i>Journal of Chemical Physics</i> , 2012 , 137, 084314	3.9	27
145	Theoretical study of the cooperative effects between the triel bond and the pnictogen bond in $\text{BF}_3\cdots\text{NCXH}_2\cdots\text{Y}$ ($\text{X} = \text{P, As, Sb; Y} = \text{H}_2\text{O, NH}_3$) complexes. <i>Journal of Molecular Modeling</i> , 2016 , 22, 10	2	26

144	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	3.7	26
143	Carbon Excess CN: A Potential Candidate as Li-Ion Battery Material. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 37135-37141	9.5	26
142	Cooperative effects between Ehole triel and Ehole chalcogen bonds.. <i>RSC Advances</i> , 2018 , 8, 26580-26588	3.7	25
141	The dual role of pnicoen as Lewis acid and base and the unexpected interplay between the pnicoen bond and coordination interaction in H ₃ N?FH ₂ X?MCN (X = P and As; M = Cu, Ag, and Au). <i>New Journal of Chemistry</i> , 2015 , 39, 2067-2074	3.6	24
140	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, 2853-8	2.8	24
139	Tuning the Competition between Hydrogen and Tetrel Bonds by a Magnesium Bond. <i>ChemPhysChem</i> , 2020 , 21, 212-219	3.2	24
138	Carbene triel bonds between TrR ₃ (Tr = B, Al) and N-heterocyclic carbenes. <i>International Journal of Quantum Chemistry</i> , 2019 , 119, e25867	2.1	24
137	Modulating the strength of tetrel bonding through beryllium bonding. <i>Journal of Molecular Modeling</i> , 2016 , 22, 192	2	23
136	Enhancement of iodine-hydride interaction by substitution and cooperative effects in NCX-NCI-HMY complexes. <i>ChemPhysChem</i> , 2012 , 13, 3997-4002	3.2	23
135	Interplay between the Etetrel bond and Ehalogen bond in PhSiF ₃ ?4-iodopyridine?N-base. <i>RSC Advances</i> , 2017 , 7, 21713-21720	3.7	22
134	Abnormal synergistic effects between Lewis acid?base interaction and halogen bond in F ₃ B?NCX?NCM. <i>Molecular Physics</i> , 2015 , 113, 3809-3814	1.7	22
133	The single-electron hydrogen, lithium, and halogen bonds with HBe, H ₂ B, and H ₃ C radicals as the electron donor: an ab initio study. <i>Structural Chemistry</i> , 2012 , 23, 411-416	1.8	22
132	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	2.1	22
131	Theoretical study on the cooperativity of hydrogen bonds in (HNC) ₂ ?HF complexes. <i>Computational and Theoretical Chemistry</i> , 2009 , 896, 112-115		22
130	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, 2432-40	3.5	21
129	Synergistic and diminutive effects between triel bond and regium bond: Attractive interactions between Ehole and Ehole. <i>Applied Organometallic Chemistry</i> , 2019 , 33, e4806	3.1	21
128	Comparison for Ehole and Ehole tetrel-bonded complexes involving cyanoacetaldehyde. <i>Molecular Physics</i> , 2018 , 116, 222-230	1.7	20
127	Competition between dihydrogen bond and beryllium bond in complexes between HBeH and HArF: a huge blue shift of distant H-Ar stretch. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 90, 135-40	4.4	20

126	Competition between hydrogen bonds and halogen bonds in complexes of formamidine and hypohalous acids. <i>Journal of Molecular Modeling</i> , 2013 , 19, 4529-35	2	20
125	The effect of methyl group on the cooperativity between three types of hydrogen bond: O?H...O, C?H...O, and O?H...N. <i>International Journal of Quantum Chemistry</i> , 2008 , 108, 558-566	2.1	20
124	Prominent enhancing effects of substituents on the strength of hydrogen tetrel bond. <i>International Journal of Quantum Chemistry</i> , 2017 , 117, e25448	2.1	19
123	Prediction and characterization of HCCH...AuX (X = OH, F, Cl, Br, CH ₃ , CCH, CN, and NC) complexes: a Au-bond. <i>Journal of Chemical Physics</i> , 2011 , 135, 074304	3.9	19
122	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, 9153-60	3.6	18
121	A new interaction mechanism of LiNH ₂ with MgH ₂ : magnesium bond. <i>Journal of Molecular Modeling</i> , 2013 , 19, 247-53	2	18
120	Comparison of tetrel bonds and halogen bonds in complexes of DMSO with ZF ₃ X (Z = C and Si; X = halogen). <i>RSC Advances</i> , 2016 , 6, 79245-79253	3.7	18
119	Comparison of Hydrogen Tetrel Bonds between TH F/F TO and H CX (X=O, S, Se). <i>ChemPhysChem</i> , 2019 , 20, 627-635	3.2	18
118	How do organic gold compounds and organic halogen molecules interact? Comparison with hydrogen bonds. <i>RSC Advances</i> , 2015 , 5, 12488-12497	3.7	17
117	Comparison for E-hole and E-hole tetrel-bonded complexes involving F ₂ CCFTF ₃ (T = C, Si, and Ge): Substitution, hybridization, and solvation effects. <i>Journal of Fluorine Chemistry</i> , 2018 , 207, 38-44	2.1	16
116	Large blue shift of the H-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, 506-11	4.4	16
115	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	4.4	15
114	Regulation of coin metal substituents and cooperativity on the strength and nature of tetrel bonds. <i>RSC Advances</i> , 2017 , 7, 46321-46328	3.7	14
113	Competition between E-hole pnictogen bond and E-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	14
112	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	3.9	14
111	Influence of the protonation of pyridine nitrogen on pnictogen bonding: competition and cooperativity. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 11348-56	3.6	14
110	Comparison of E-hole and E-hole tetrel bonds in complexes of borazine with TH ₃ F and F ₂ TO/H ₂ TO (T = C, Si, Ge). <i>International Journal of Quantum Chemistry</i> , 2019 , 119, e25910	2.1	14
109	Interplay between metal-π interactions and hydrogen bonds: some unusual synergetic effects of coinage metals and substituents. <i>ChemPhysChem</i> , 2013 , 14, 3341-7	3.2	13

108	What is the role of defects in single-walled carbon nanotubes for nonlinear optical property? <i>Journal of Materials Chemistry</i> , 2011 , 21, 8905		13
107	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. <i>Journal of Computational Chemistry</i> , 2010 , 31, 1662-9	3.5	13
106	TrielHydride triel bond between ZX ₃ (Z = B and Al; X = H and Me) and THMe ₃ (T = Si, Ge and Sn). <i>Applied Organometallic Chemistry</i> , 2018 , 32, e4367	3.1	13
105	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	12
104	Comparison between Hydrogen and Halogen Bonds in Complexes of 6-OX-Fulvene with Pnicogen and Chalcogen Electron Donors. <i>ChemPhysChem</i> , 2019 , 20, 1978-1984	3.2	12
103	A dual-functional fluorescent probe for sequential determination of Cu/S and its applications in biological systems. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020 , 243, 118797	4.4	12
102	Tetrel Bond between 6-OTXEFulvene and NHSubstituents and Aromaticity. <i>Molecules</i> , 2018 , 24,	4.8	11
101	Influence of substituents on the nature of metalπ interaction and its cooperativity with halogen bond. <i>Journal of Chemical Physics</i> , 2015 , 143, 054308	3.9	11
100	Theoretical study on garmylenoid H ₂ GeFBeF. <i>Structural Chemistry</i> , 2012 , 23, 867-871	1.8	11
99	Partially covalent nature and substitution non-additivity of Au-bonding in H ₂ OAuCH ₃ complex. <i>Chemical Physics Letters</i> , 2010 , 498, 259-262	2.5	11
98	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020 , 228, 117763	4.4	11
97	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	7.3	11
96	Non-additivity between substitution and cooperative effects in enhancing hydrogen bonds. <i>Journal of Chemical Physics</i> , 2014 , 141, 244305	3.9	10
95	Effect of substitution and cooperativity on the Clπ blue shift in single-electron halogen-bonded H ₃ C ππClF complex. <i>Molecular Physics</i> , 2010 , 108, 2021-2026	1.7	10
94	Solvent effect on the role of methyl groups in formation of OππHO hydrogen bond in dimethyl etherπmethanol complex. <i>Computational and Theoretical Chemistry</i> , 2008 , 862, 74-79		10
93	Coinage metal dimers as the noncovalent interaction acceptors: study of the Elump interactions. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 21152-21161	3.6	9
92	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 , 115, 99-105	2.1	9
91	Coinage-Metal Bond between [1.1.1]Propellane and M/MCl/MCH (M = Cu, Ag, and Au): Cooperativity and Substituents. <i>Molecules</i> , 2019 , 24,	4.8	9

- 90 Substitution reactions of $H_2GeFBeF$ with RH ($R = F, OH, NH_2$): A theoretical study. *Russian Journal of Physical Chemistry A*, **2014**, 88, 1097-1102 0.7 9
- 89 Competitive interaction between halogen and hydrogen bonds in $NH_2Br-HOX$ ($X = F, Cl, \text{ and } Br$) complex. *International Journal of Quantum Chemistry*, **2012**, 112, 2429-2434 2.1 9
- 88 Synergistic and Diminutive Effects between Regium and Aerogen Bonds. *ChemPhysChem*, **2020**, 21, 2426-2431 3.2 9
- 87 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
- 86 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
- 85 The Hole tetrel bond between X_2TO and CO_2 : Substituent effects and its potential adsorptivity for CO_2 . *International Journal of Quantum Chemistry*, **2020**, 120, e26251 2.1 8
- 84 Dinuclear first-row transition metal(C_8Me_6) $_2$ 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
- 83 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
- 82 THEORETICAL INVESTIGATION ON THE INSERTION REACTIONS OF THE GERMYLENOID $H_2GeLiFWITHRH$ ($R=Cl,SH,PH_2$). *Journal of Theoretical and Computational Chemistry*, **2013**, 12, 1350003 1.8 8
- 81 Bioinspired surface with special wettability for liquid transportation and separation. *Sustainable Materials and Technologies*, **2020**, 25, e00175 5.3 7
- 80 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
- 79 Abnormal Tetrel Bonds between Formamidine and TH_3F : Substituent Effects. *ChemistrySelect*, **2018**, 3, 2842-2849 1.8 7
- 78 The ability of a tetrel bond to transition a neutral amino acid into a zwitterion. *Chemical Physics Letters*, **2019**, 731, 136584 2.5 7
- 77 The structure, properties, and nature of CBr_2F halogen bond involving $HArF$: Substitution, hybridization, and nonadditivity. *Journal of Fluorine Chemistry*, **2012**, 135, 207-212 2.1 7
- 76 Influence of cooperativity on the frequency shift of the ArH stretch vibration in $HArF$ complexes. *Molecular Physics*, **2013**, 111, 497-504 1.7 7
- 75 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
- 74 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
- 73 Beryllium decorated armchair BC_2N nanoribbons: coexistence of planar tetracoordinate carbon and nitrogen moieties. *RSC Advances*, **2015**, 5, 73945-73950 3.7 6

72	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	2.8	6
71	Is a MH (M = Be and Mg) radical a better electron donor in halogen-hydride interaction?: A theoretical comparison with HMH. <i>International Journal of Quantum Chemistry</i> , 2013 , 113, 1293-1298	2.1	6
70	Intramolecular Si-O-Tetrel Bonding: Tuning of Substituents and Cooperativity. <i>ChemistrySelect</i> , 2017 , 2, 11104-11112	1.8	6
69	Complicated synergistic effects between metal-π interaction and halogen bonding involving MCCX. <i>RSC Advances</i> , 2015 , 5, 105160-105168	3.7	6
68	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	3.7	6
67	Theoretical study on the insertion reactions of the germylenoid H ₂ GeClMgCl with RH (R = F, OH, NH ₂). <i>Russian Journal of Physical Chemistry A</i> , 2012 , 86, 1969-1973	0.7	6
66	Effect of superalkali substituents on the strengths and properties of hydrogen and halogen bonds. <i>Journal of Molecular Modeling</i> , 2013 , 19, 1311-8	2	6
65	The prominent enhancing effect and mechanism of the methyl group in the X ⁺ ...Y (X=O, S, H ₃ CO, H ₃ CS, (H ₃ C) ₂ O, (H ₃ C) ₂ S; Y=HCN, HNC) hydrogen-bonded complex. <i>Molecular Physics</i> , 2011 , 109, 831-838	1.7	6
64	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 84, 68-73	4.4	6
63	Comparison of halide donors based on π-M (M = Cu, Ag, Au), π-H and π-halogen bonds. <i>Theoretical Chemistry Accounts</i> , 2018 , 137, 1	1.9	6
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