Theoretical research of multipolymers with hydrogen bonds (II)

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It is a kind of work about how the properties of multipolymers with hydrogen bonds changed. In this article, applying the HF, H_2O, NH_3 and CH_4, a series of characters of tripolymers, such as ESP, ELF, AIM, etc. have been observed. There are several results after calculations.

Computational details:

Geometry and frequency: M06-2X/6-311G** with "int=ultrafine" in Gaussian 09 D.01 program package

Wavefunction analysis: Multiwfn 3.6 (dev)

Isosurface plot: VMD 1.9.2

Results:

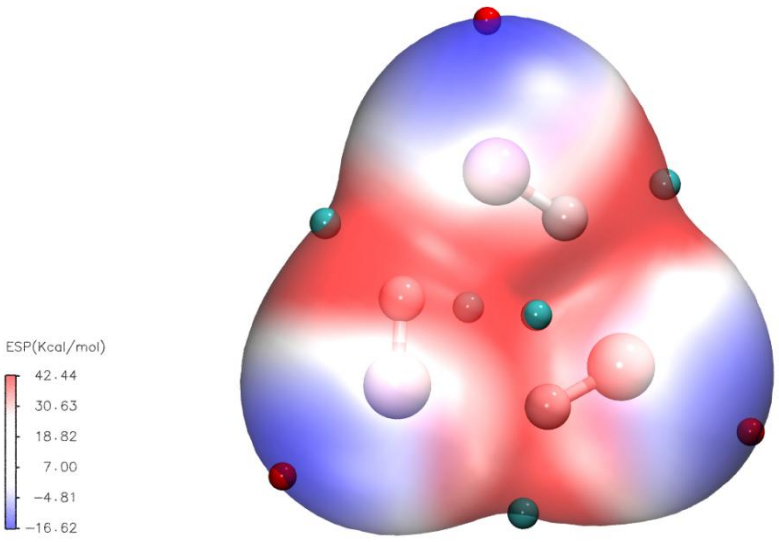
1. Average Interaction Energy

	$(HF)_3$	$(H_2O)_3$	$(NH3)_3$	$(CH_4)_3$
E_int(Kcal/mol)	8.07	7.93	5.63	0.42
Symmetry	C_{3h}	C_3	C_{3h}	C_{3h}

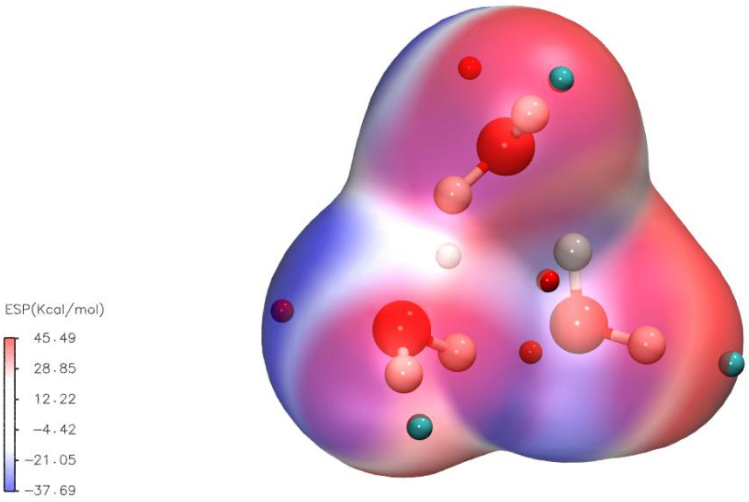
2. ESP: Electrostatic Potential

PS: a novel method of plotting ESP with .cub files can be seen in the appendix (in Chinese).

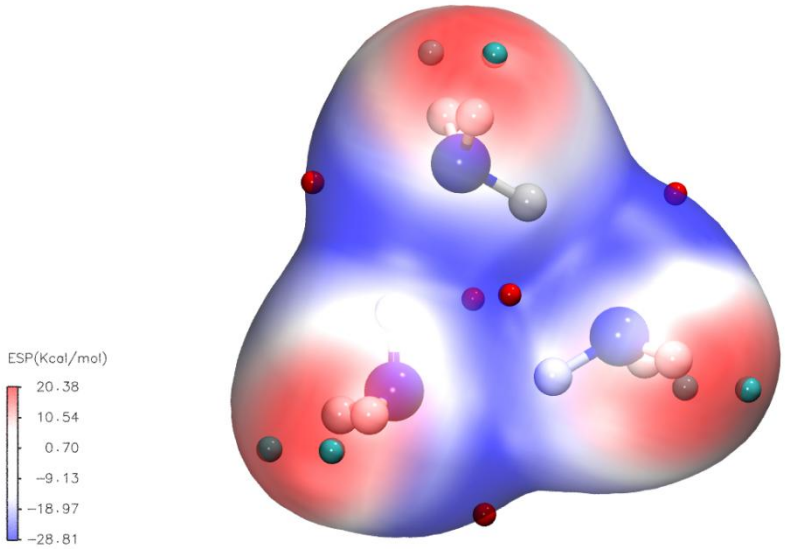
(1). ESP of $(HF)_3$



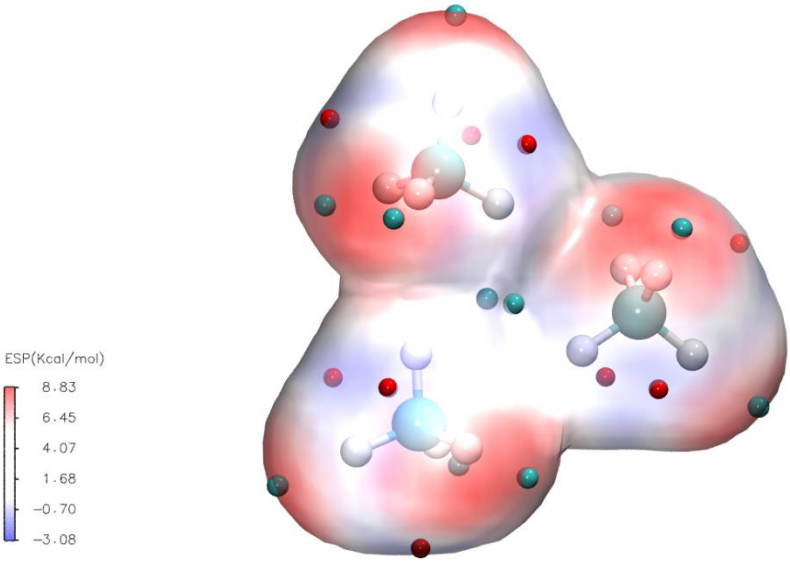
(2). ESP of $(H_2O)_3$



(3). ESP of $(NH_3)_3$

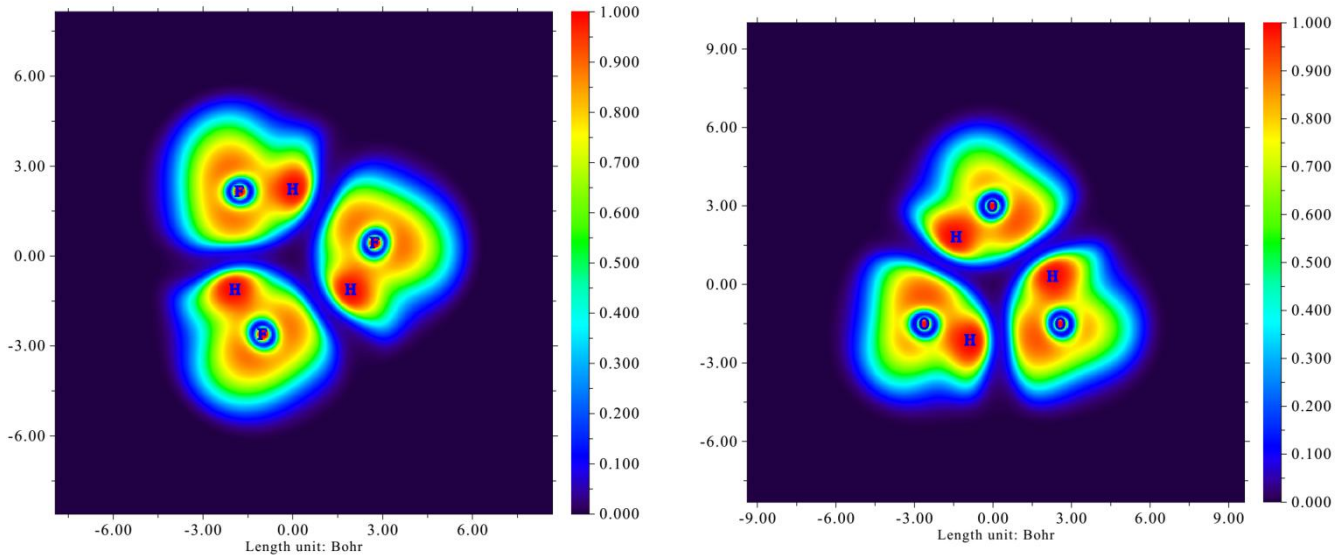


(4). ESP of $(CH_4)_3$

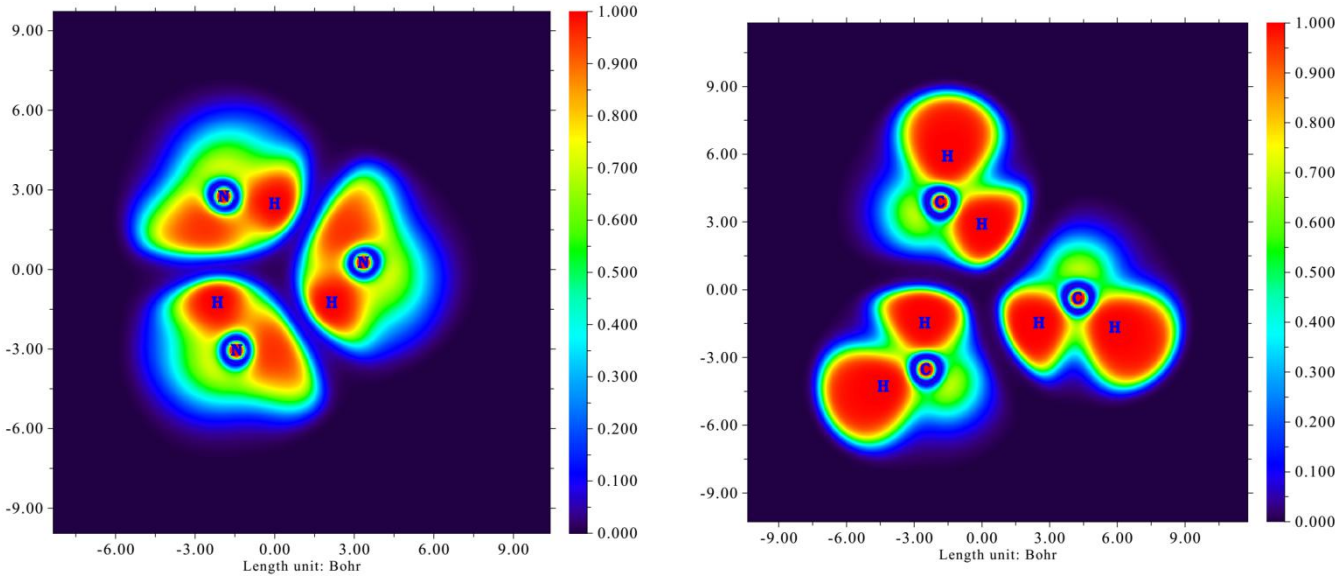


3. ELF: Electron Localization Function

(1). ELF of $(HF)_3$ (left) and ELF of $(H_2O)_3$ (right)



(2). ELF of $(NH_3)_3$ (left) and ELF of $(CH_4)_3$ (right)



4. Mayer bond order and Multicenter bond order

Mayer	$(HF)_3$	$(H_2O)_3$	$(NH3)_3$	$(CH_4)_3$
H-X…H	0.091	0.105	0.119	0.002
Multicenter	**$(HF)_3$**	**$(H_2O)_3$**	**$(NH3)_3$**	**$(CH_4)_3$**
X-X-X	0.020	0.049	0.028	-0.020

*X=F, O, N and C

5. AIM topology analysis

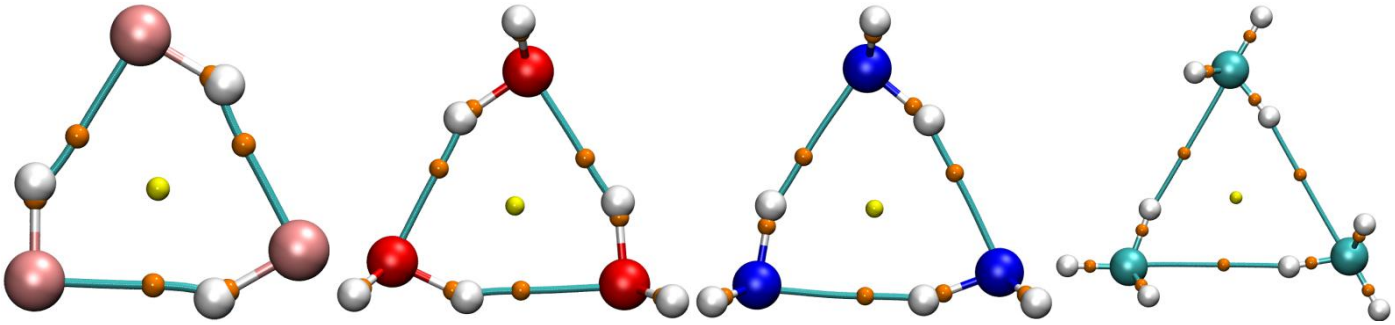
(1). Several properties of CPs are listed in the table below.

Tripolymers	$(HF)_3$		$(H_2O)_3$		$(NH3)_3$		$(CH_4)_3$	
Kind of Critical Point (CP)	BCP	RCP	BCP	RCP	BCP	RCP	BCP	RCP
Lagrangian kinetic energy G(r)	3.51E-02	1.32E-02	2.71E-02	9.52E-03	1.59E-02	5.55E-03	3.22E-03	1.42E-03
Hamiltonian kinetic energy K(r)	3.59E-04	-2.45E-03	-1.45E-03	-1.65E-03	-1.91E-03	-1.06E-03	-7.63E-04	-4.67E-04
Potential energy density V(r)	-3.54E-02	-1.07E-02	-2.57E-02	-7.87E-03	-1.40E-02	-4.49E-03	-2.46E-03	-9.57E-04
Energy density E(r) or H(r)	-3.59E-04	2.45E-03	1.45E-03	1.65E-03	1.91E-03	1.06E-03	7.63E-04	4.67E-04
Laplacian of electron density	1.39E-01	6.25E-02	1.14E-01	4.47E-02	7.11E-02	2.64E-02	1.59E-02	7.56E-03
Electron localization function (ELF)	7.80E-02	1.09E-02	8.05E-02	1.33E-02	7.80E-02	1.21E-02	1.43E-02	4.17E-03
Localized orbital locator (LOL)	2.25E-01	9.52E-02	2.28E-01	1.04E-01	2.25E-01	9.98E-02	1.08E-01	6.12E-02
Local information entropy	7.67E-03	2.72E-03	6.79E-03	2.42E-03	5.10E-03	1.78E-03	1.39E-03	6.47E-04
Reduced density gradient (RDG)	1.34E-16	1.48E-14	3.05E-16	7.33E-16	6.50E-16	4.45E-16	1.74E-16	8.38E-16
Sign(lambda2)*rho	-3.39E-02	1.02E-02	-2.94E-02	8.93E-03	-2.11E-02	6.29E-03	-4.77E-03	2.02E-03
Average local ionization energy	7.24E-01	7.46E-01	5.89E-01	6.32E-01	4.74E-01	5.47E-01	5.23E-01	5.07E-01
Delta_g	7.72E-02	3.44E-02	5.74E-02	2.63E-02	3.21E-02	1.82E-02	1.53E-02	6.70E-03
Total ESP	2.94E-01	1.26E-01	1.63E-01	3.61E-02	4.33E-02	-2.56E-02	2.11E-02	4.54E-03
Ellipticity of electron density	9.91E-03	-1.32E+00	7.85E-02	-1.32E+00	9.05E-02	-1.33E+00	1.09E-01	-1.31E+00
eta index	2.18E-01	3.16E-01	2.16E-01	3.23E-01	2.10E-01	3.35E-01	1.22E-01	3.05E-01

*BCP = Bond Critical Point; RCP = Ring Critical Point

(2) . plots of AIM topology analysis

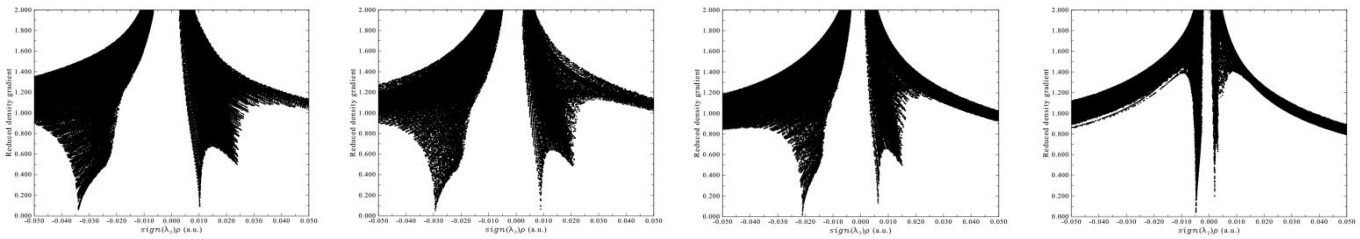
A. plots of $(HF)_3$; B. plots of $(H_2O)_3$; C.plots of $(NH_3)_3$; D. plots of of $(CH_4)_3$



6. RDG: Reduced density gradient

(1). Scatter plots

A. plots of $(HF)_3$; B. plots of $(H_2O)_3$; C.plots of $(NH_3)_3$; D. plots of of $(CH_4)_3$

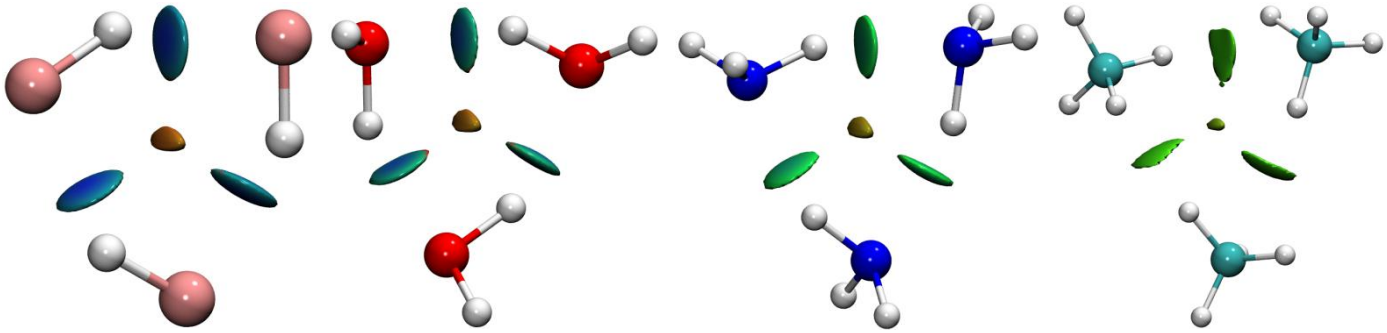


The marked scales of two cusps on the X axis are

A: **-0.035(left); 0.010(right);** B: **-0.030(left); 0.010(right);** C: **-0.021(left); 0.006(right);** D: **-0.005(left); 0.002(right);**

(2). Isosurface plots of RDG

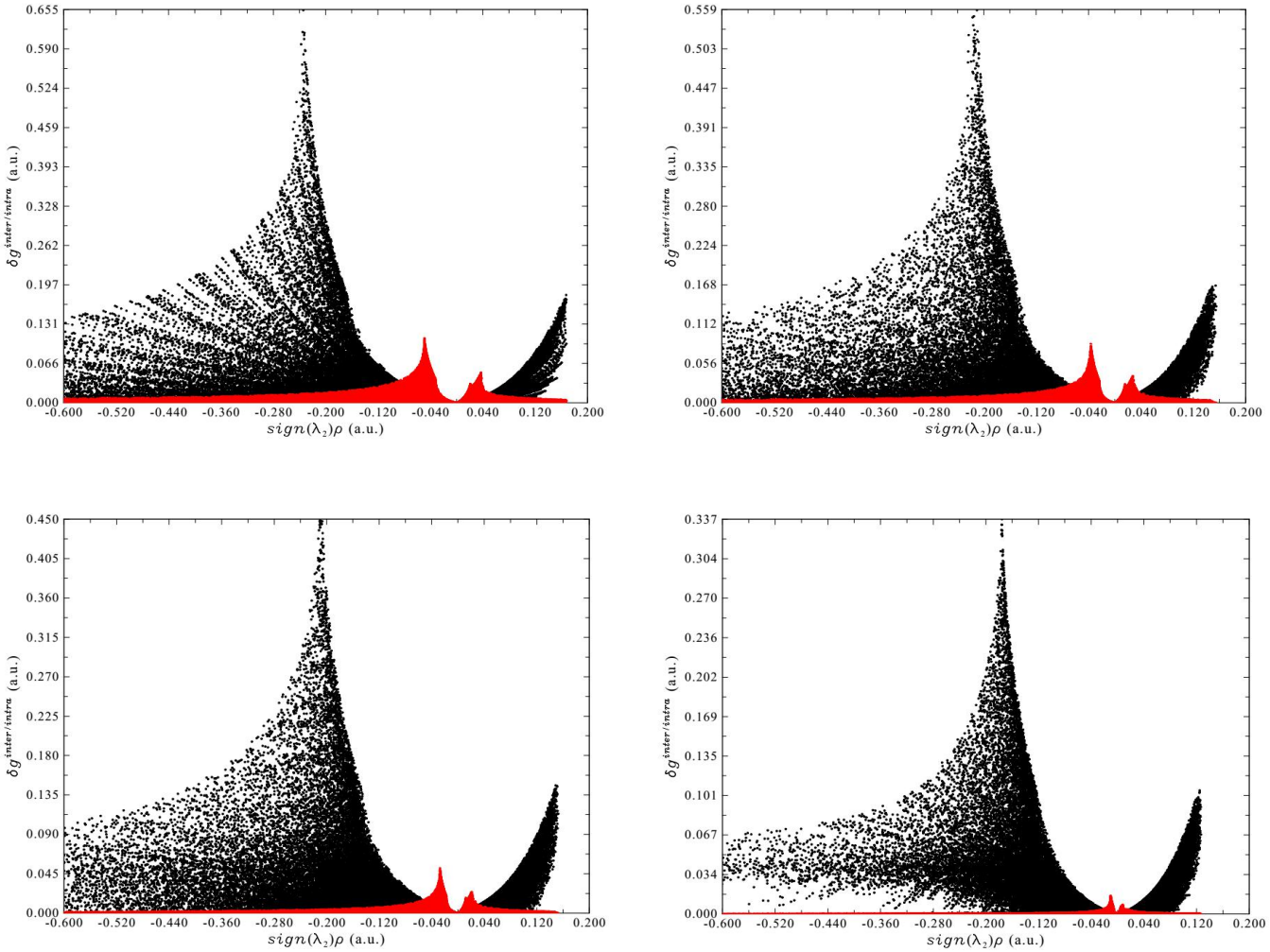
A. **plots of $(HF)_3$**; B. **plots of $(H_2O)_3$**; C.**plots of $(NH_3)_3$**; D. **plots of of $(CH_4)_3$**



7. IGM: Independent Gradient Model

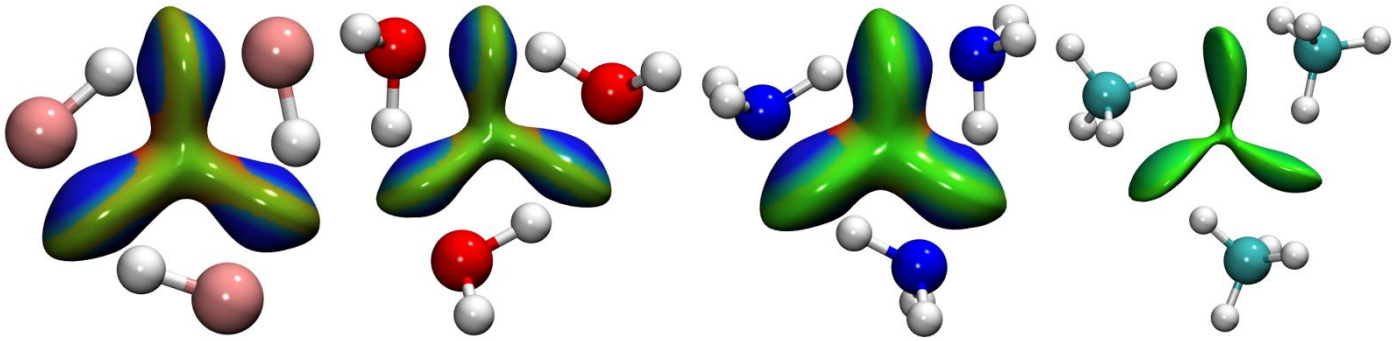
(1). Scatter plots

A. **plots of $(HF)_3$**; B. **plots of $(H_2O)_3$**; C.**plots of $(NH_3)_3$**; D. **plots of of $(CH_4)_3$**



(2). Isosurface plots of IGM

A. **plots of $(HF)_3$**; B. **plots of $(H_2O)_3$**; C.**plots of $(NH_3)_3$**; D. **plots of of $(CH_4)_3$**



*isovalue of isosurface of $(HF)_3$ and $(H_2O)_3$ are 0.015, and others are 0.005.

Conclusion

According with the original idea, the weak interaction of the system increased with the arising of atomic number of centre atoms.