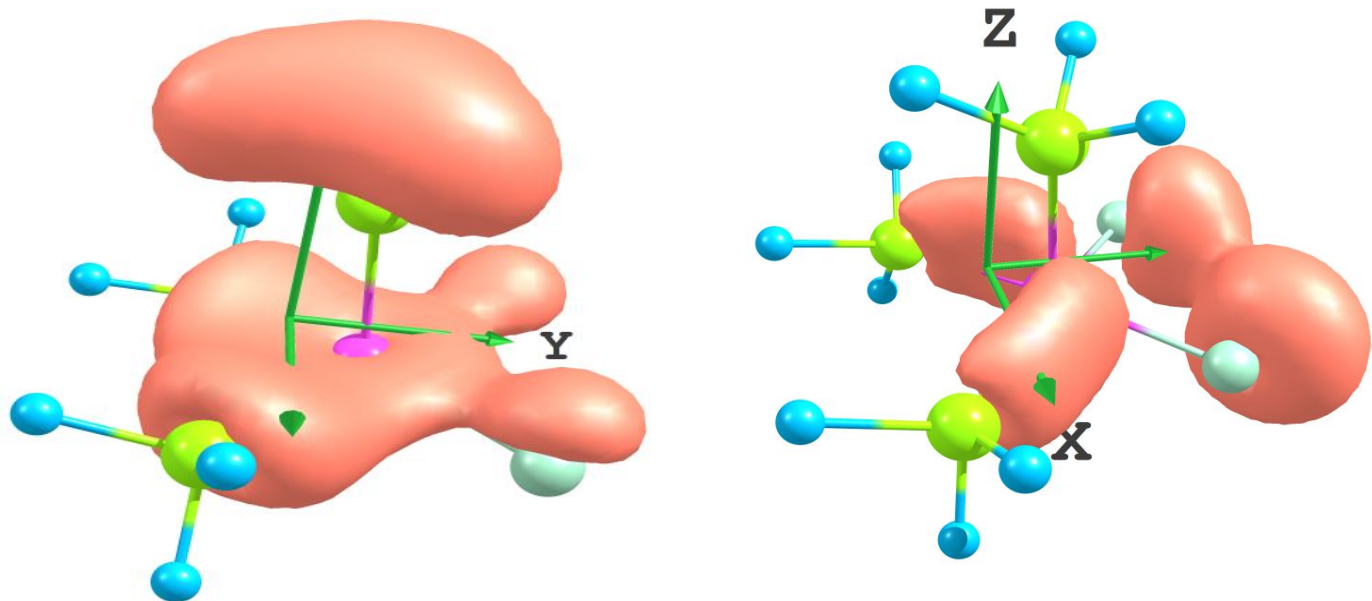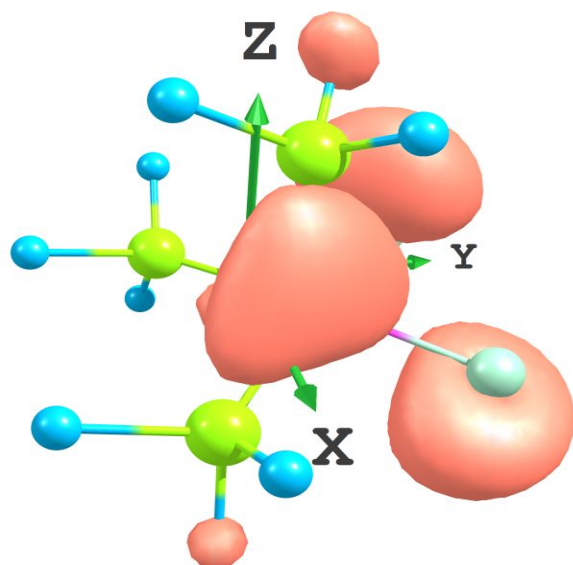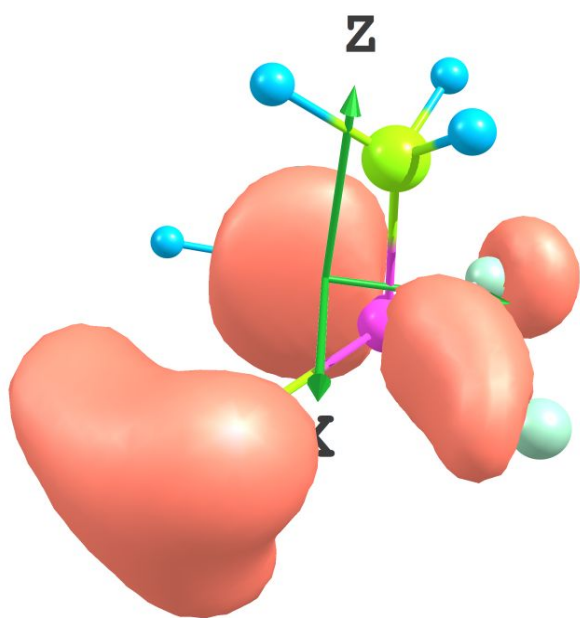In all figures, CCSD is on the left and BhandHLYP is on the right. In tables, CCSD is colored red and BHandHLYP is colored blue.

HOMO

HOMO-1

HOMO-2
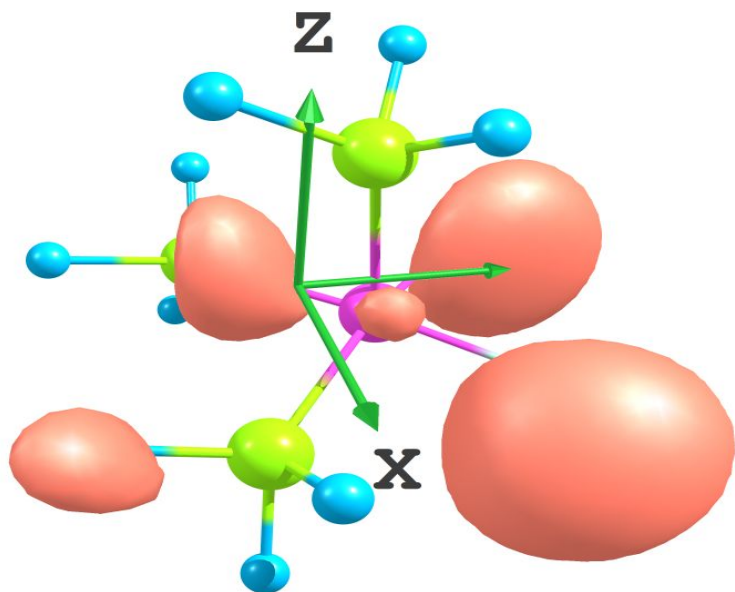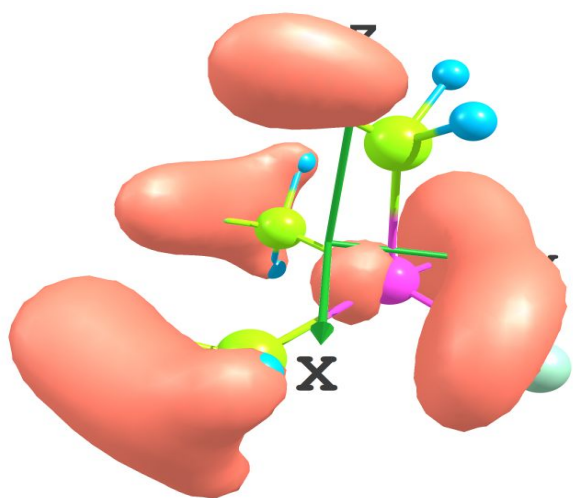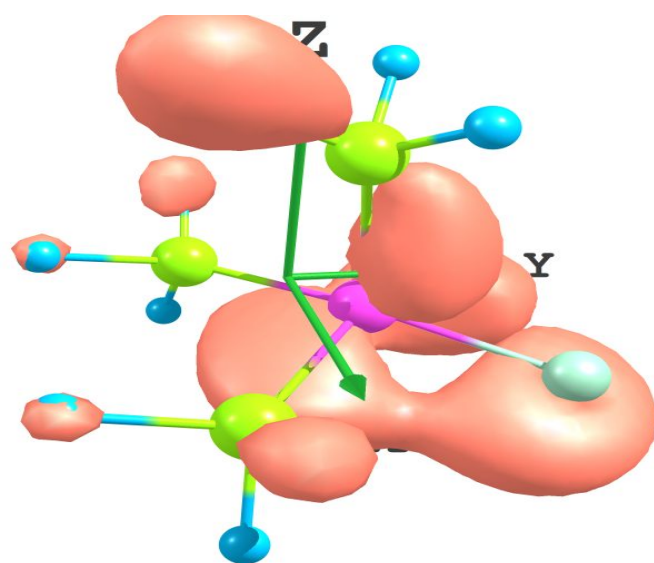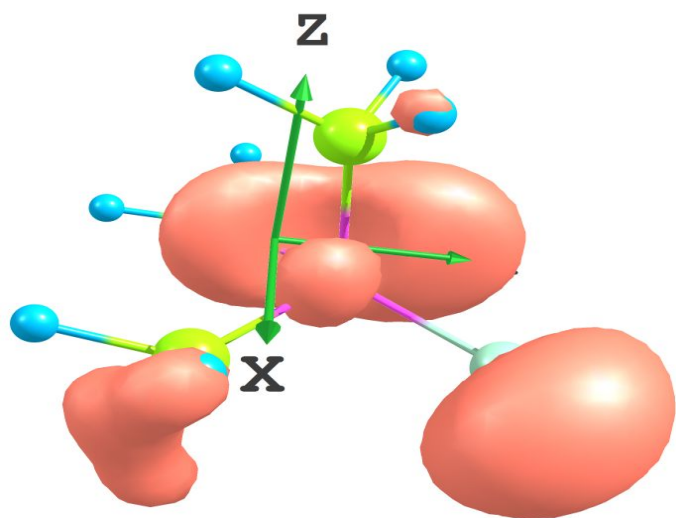
HOMO-3

HOMO-4
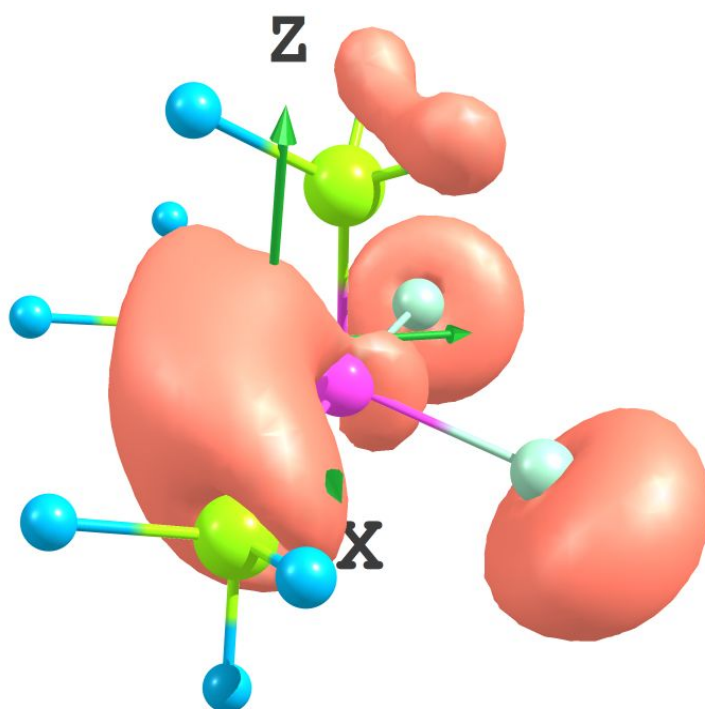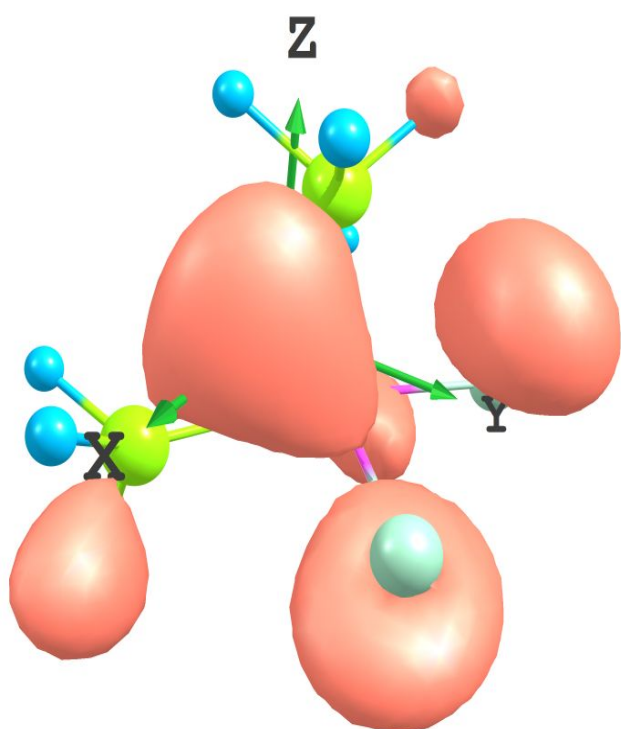
LUMO
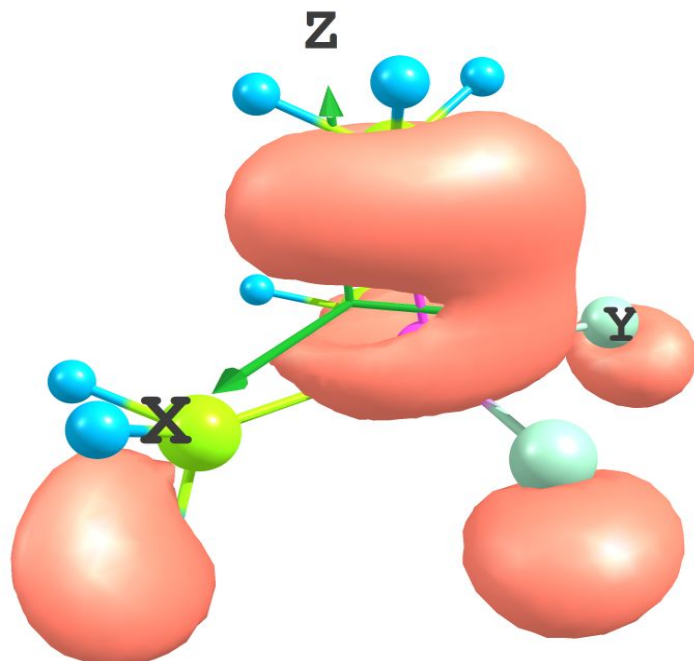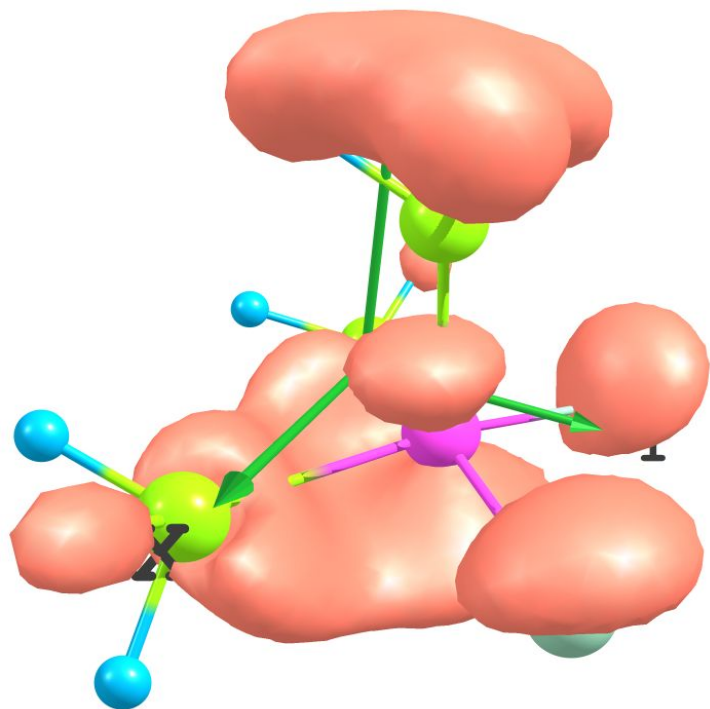
LUMO+1
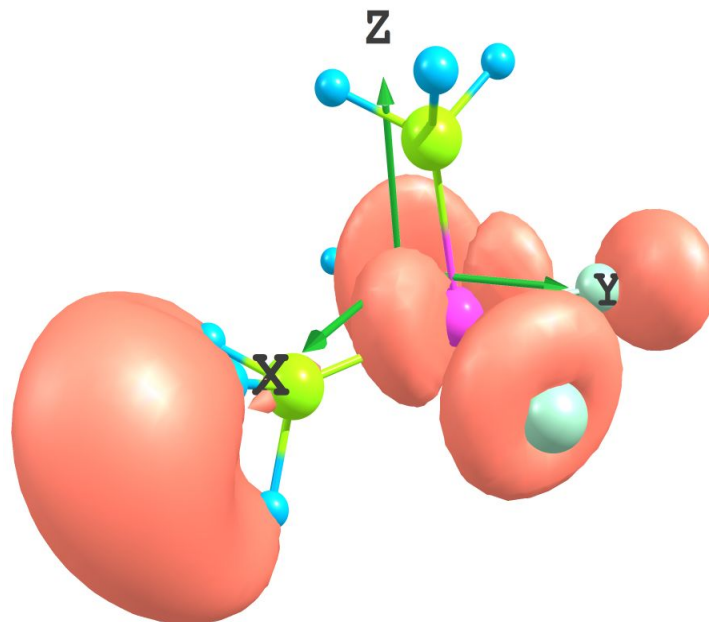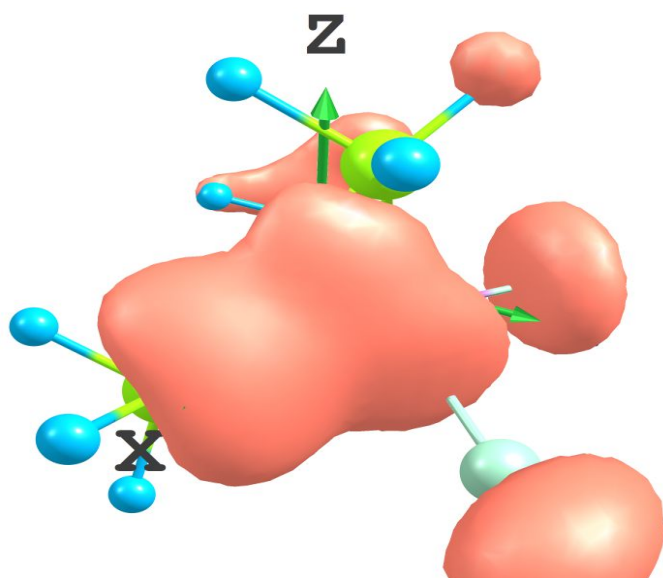
LUMO+2
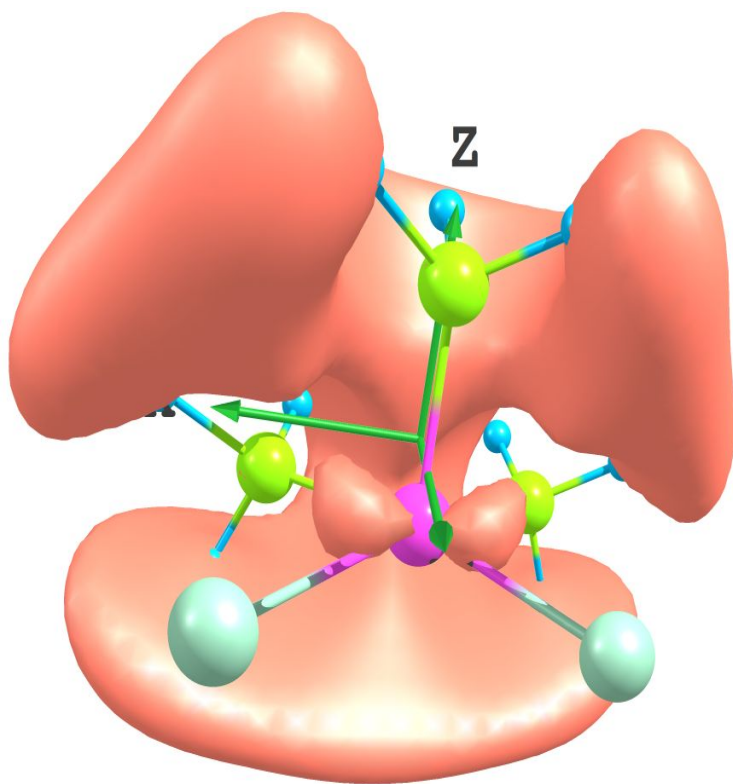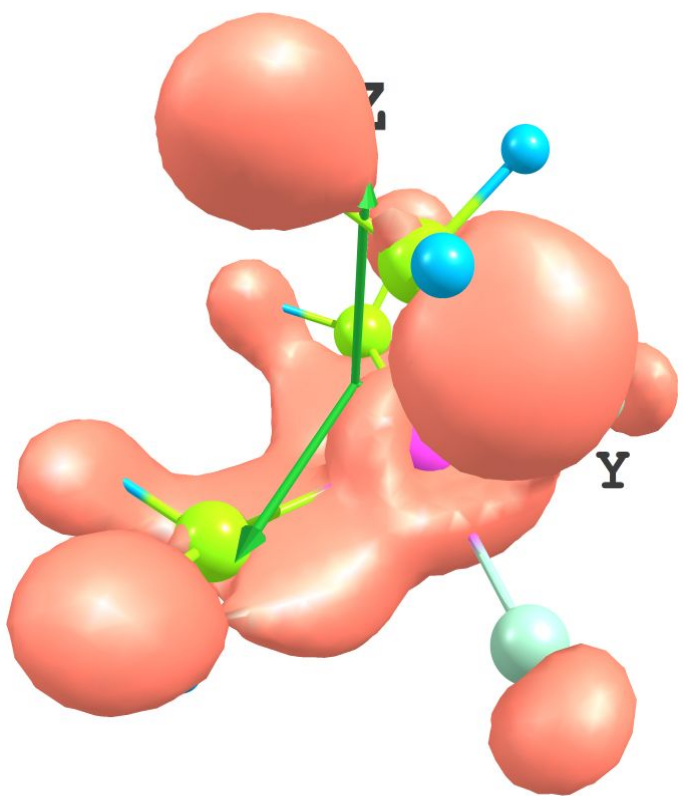
LUMO+3
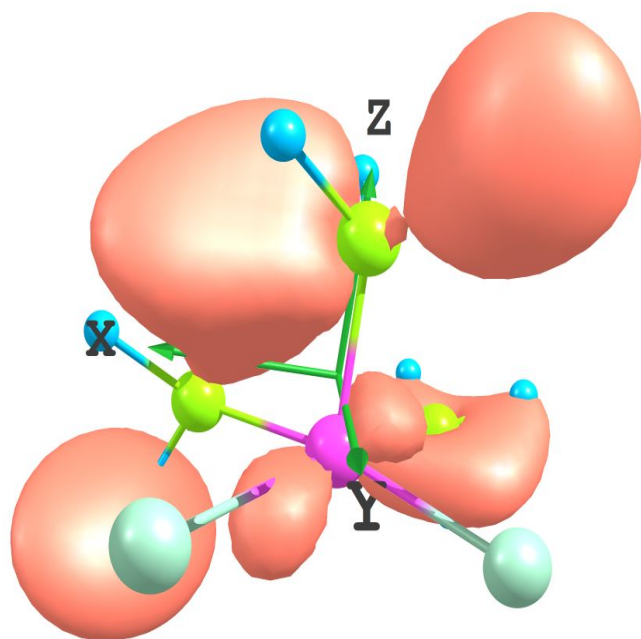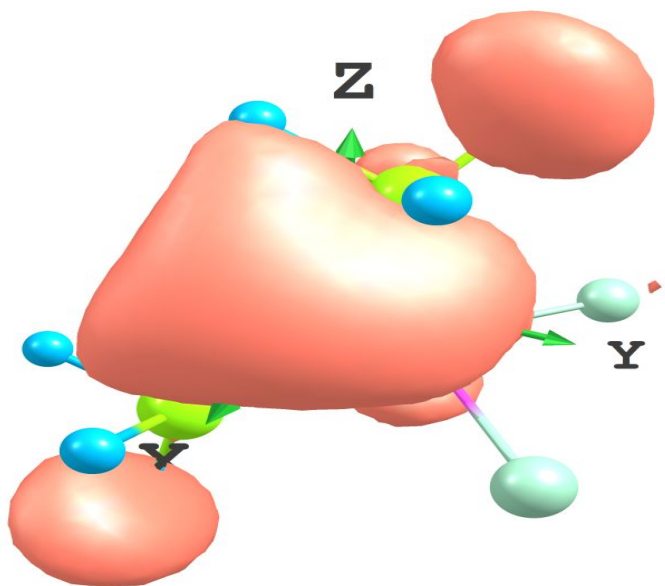
LUMO+4
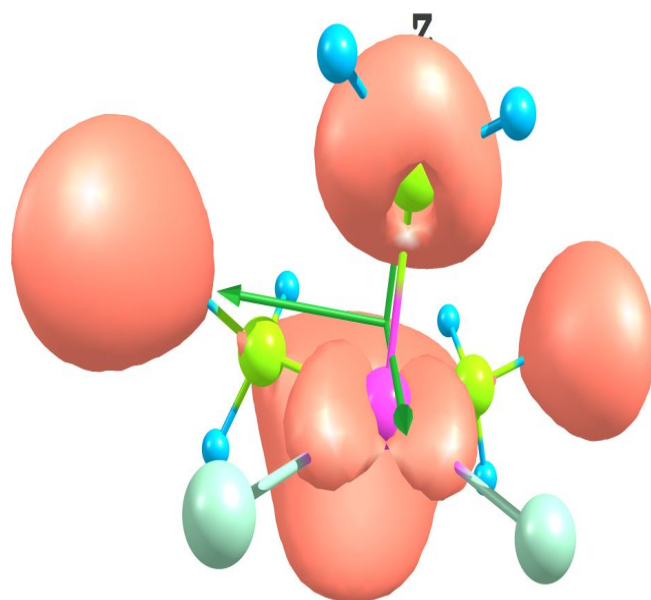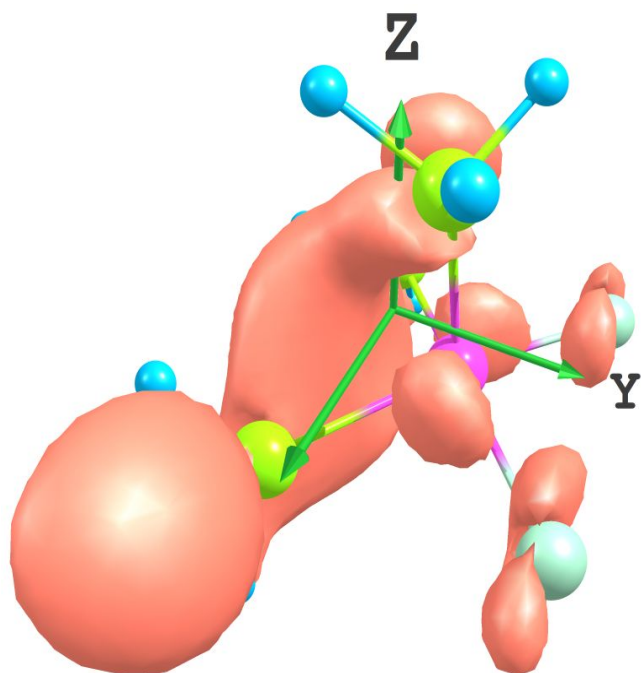
CCSD
[28 electrons found in the effective core potential]
WARNING: 4 low occupancy (<1.9990e) core orbitals found on Ru   1
        1 low occupancy (<1.9990e) core orbital found on P   3
        1 low occupancy (<1.9990e) core orbital found on P   4
        1 low occupancy (<1.9990e) core orbital found on P   6
  1   Ru 1   S   Cor(4S)   1.99005
  7   Ru 1   px   Cor(4p)   1.99364
  11   Ru 1   py   Cor(4p)   1.99534
  15   Ru 1   pz   Cor(4p)   1.98604
  79   P   3 S   Cor(2S)   1.99693
  116 P   4 S   Cor(2S)   1.99693
  190 P   6 S   Cor(2S)   1.99617

BHandHLYP
[28 electrons found in the effective core potential]
WARNING: 4 low occupancy (<1.9990e) core orbitals found on Ru   1
        1 low occupancy (<1.9990e) core orbital found on P   3
        1 low occupancy (<1.9990e) core orbital found on P   4
        1 low occupancy (<1.9990e) core orbital found on P   6

```
   1  Ru   1 S    Cor( 4S)    1.99291
   7  Ru   1 px   Cor( 4p)    1.99708
  11  Ru   1 py   Cor( 4p)    1.99825
  15  Ru   1 pz   Cor( 4p)    1.98824
  79  P    3 S    Cor( 2S)    1.99766
 116  P    4 S    Cor( 2S)    1.99766
 190  P    6 S    Cor( 2S)    1.99693
```

<p style="text-align:center;color:red;">Natural Population CCSD</p>

```
-----------------------------------------------------------
  Effective Core          28.00000
  Core                    57.95100 ( 99.9155% of  58)
  Valence                 45.09519 ( 98.0330% of  46)
  Natural Minimal Basis   131.04619 ( 99.2774% of 132)
  Natural Rydberg Basis     0.95381 (  0.7226% of 132)
-----------------------------------------------------------
```

<p style="text-align:center;color:blue;">Natural Population BHandHLYP</p>

```
-----------------------------------------------------------
  Effective Core          28.00000
  Core                    57.96543 ( 99.9404% of  58)
  Valence                 45.76277 ( 99.4843% of  46)
  Natural Minimal Basis   131.72820 ( 99.7941% of 132)
  Natural Rydberg Basis     0.27180 (  0.2059% of 132)
```

```
Atom  No        Natural Electron Configuration
```
Red is CCSD and blue is BHandHLYP

```
---------------------------------------------------------------------------
  Ru   1    [core]5S( 0.43)4d( 7.68)5p( 0.96)4f( 0.03)5d( 0.07)6p( 0.01)6d( 0.01)
  Ru   1    [core]5S( 0.42)4d( 7.78)5p( 0.91)5d( 0.02)
  Cl   2    [core]3S( 1.84)3p( 5.37)4S( 0.01)3d( 0.10)4p( 0.03)4f( 0.01)
  Cl   2    [core]3S( 1.86)3p( 5.50)3d( 0.01)
  P    3    [core]3S( 1.27)3p( 2.98)3d( 0.09)4p( 0.02)4f( 0.01)
  P    3    [core]3S( 1.31)3p( 3.04)3d( 0.05)4p( 0.01)
  P    4    [core]3S( 1.27)3p( 2.98)3d( 0.09)4p( 0.02)4f( 0.01)
  P    4    [core]3S( 1.31)3p( 3.04)3d( 0.05)4p( 0.01)
  Cl   5    [core]3S( 1.84)3p( 5.37)4S( 0.01)3d( 0.10)4p( 0.03)4f( 0.01)
  Cl   5    [core]3S( 1.86)3p( 5.50)3d( 0.01)
  P    6    [core]3S( 1.21)3p( 2.88)3d( 0.10)4p( 0.02)4f( 0.01)
  P    6    [core]3S( 1.24)3p( 2.94)3d( 0.06)4p( 0.01)
```

Moving to Lumo
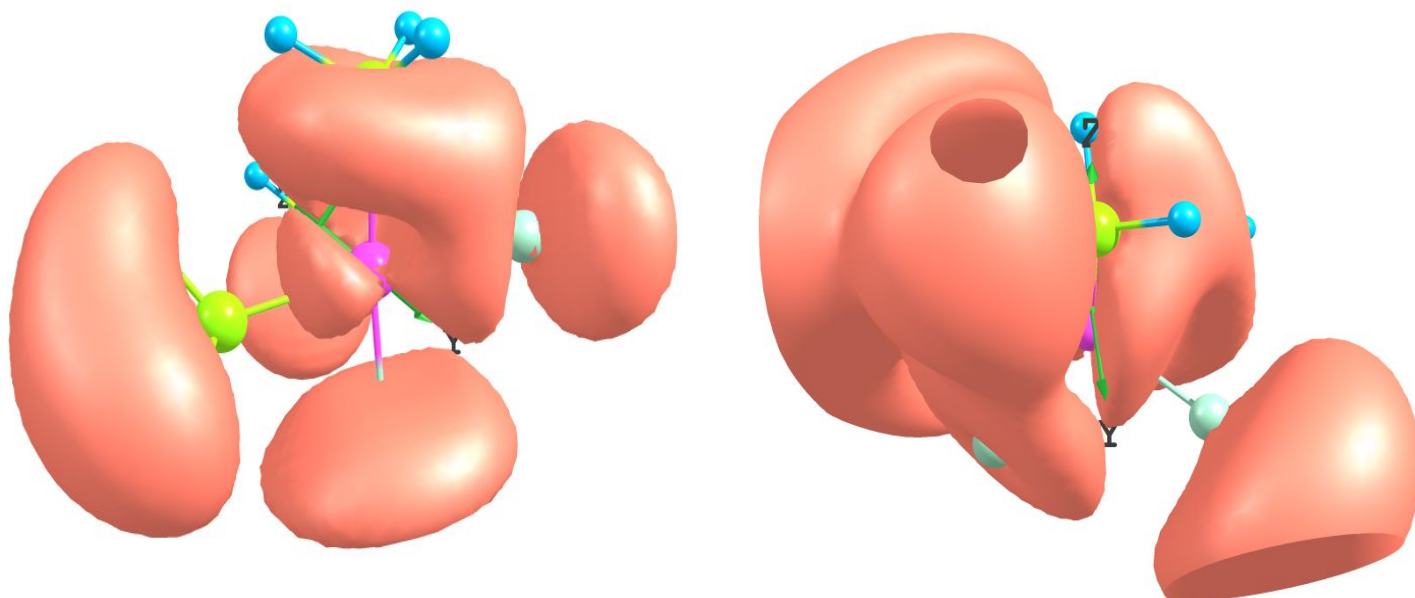
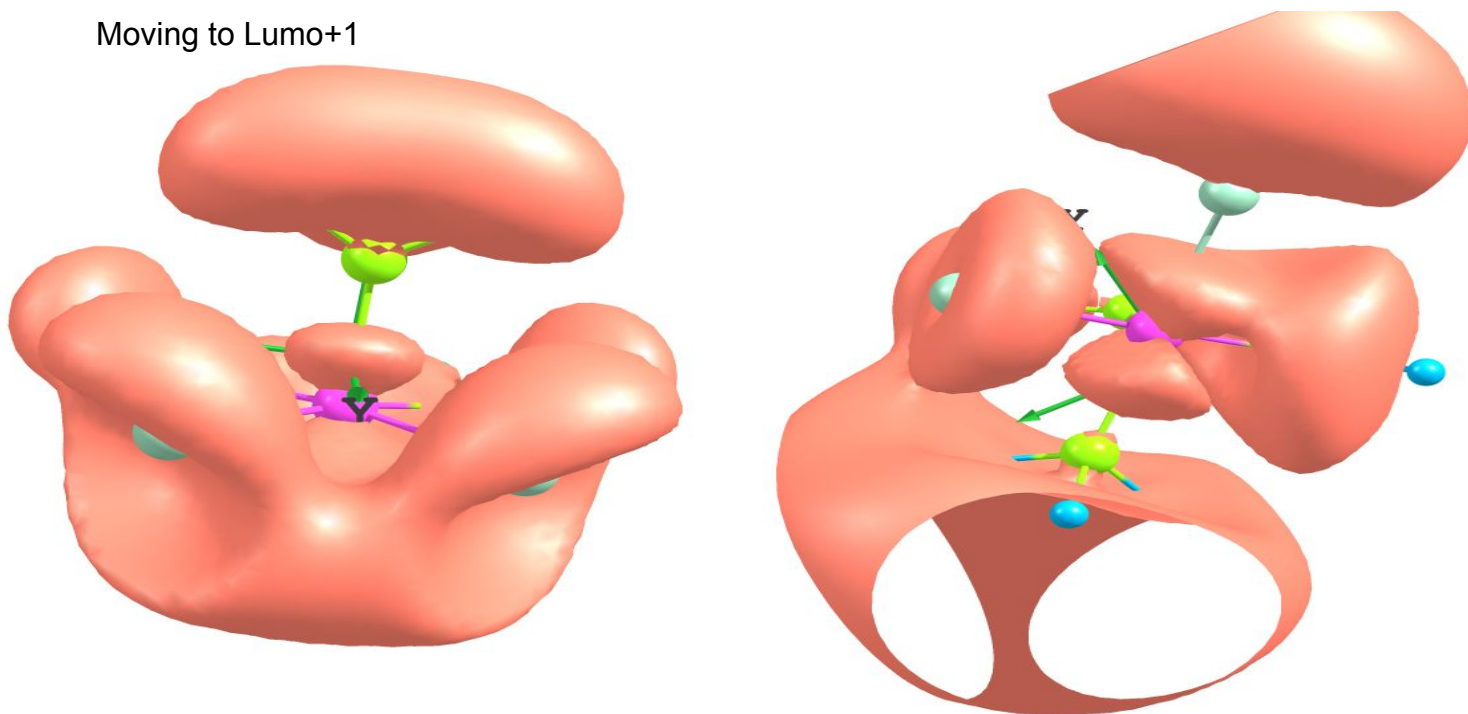| Atom	No	Natural Electron Configuration Red is CCSD and blue is BHandHLYP	
Ru	1	[core]5S(0.0)4d(0.44)5p(0.04)5d(0.01)	
Ru	1	[core]5S(0.02)4d(0.41)5p(0.13)6S(0.01)5d(0.0) beta does not have 6s	
Cl	2	[core]3S(0.0)3p(0.04)3d(0.01)4p(0.01)	beta has no 3d and 4p
Cl	2	[core]3S(0.0)3p(0.04)	
P	3	[core]3S(0.01)3p(0.04)3d(0.01)	
P	3	[core]3S(0.0)3p(0.03)3d(0.01)4p(0.01)	beta does not have 4p
P	4	[core]3S(0.04)3p(0.04)3d(0.0)	
P	4	[core]3S(0.0)3p(0.03)3d(0.01)4p(0.01)	beta does not have 4p
Cl	5	[core]3S(0.0)3p(0.05)3d(0.01)4p(0.01)	beta has no 3d and 4p
Cl	5	[core]3S(0.0)3p(0.04)	
P	6	[core]3S(0.07)3p(0.13)3d(0.0)	
P	6	[core]3S(0.06)3p(0.1)3d(0.0)4p(0.02)	beta does not have 4p
H	7	1S(0.0)	
H	7	1S(0.01)	
H	8	1S(0.0)	
H	8	1S(0.01)	
H	9	1S(0.01)	
H	9	1S(0.01)	
H	10	1S(0.01)	
H	10	1S(0.01)	
H	11	1S(0.00)	
H	11	1S(0.00)	
H	12	1S(0.01)	
H	12	1S(0.02)	
H	13	1S(0.00)	
H	13	1S(0.00)	

Moving to Lumo+1

Atom No   Natural Electron Configuration Red is CCSD and blue is BHandHLYP

Ru   1   [core]5S(0.21)4d(0.42)5p(0.02)5d(0.0)6p(0.01)   beta has no 6p
Ru   1   [core]5S(0.0)4d(0.37)5p(0.0)5d(0.0)
Cl   2   [core]3S(0.02)3p(0.10)4S(0.01)3d(0.01)   beta has no 4s and 3d
Cl   2   [core]3S(0.02)3p(0.09)3d(0.01)   no 3d in beta
P   3   [core]3S(0.05)3p(0.07)3d(0.0)
P   3   [core]3S(0.06)3p(0.05)3d(0.02)4p(0.04)   no 4p in beta
P   4   [core]3S(0.05)3p(0.08)3d(0.0)
P   4   [core]3S(0.06)3p(0.05)3d(0.02)4p(0.04)   no 4p in beta
Cl   5   [core]3S(0.02)3p(0.1)4S(0.01)3d(0.01)   beta has no 4s and
3d
Cl   5   [core]3S(0.02)3p(0.09)3d(0.01)   no 3d in beta
P   6   [core]3S(0.0)3p(0.01)3d(0.0)
P   6   [core]3S(0.0)3p(0.0)3d(0.0)
H   7   1S(0.01)
H   7   1S(0.01)
H   8   1S(0.01)

```
H   8        1S( 0.01)
H   9        1S( 0.0)
H   9        1S( 0.00)
H   10       1S( 0.01)
H   10       1S( 0.01)2S( 0.01)                          no 2s in beta
H   11       1S( 0.00)
H   11       1S( 0.01)2S( 0.01)                          no 2s in beta
H   12       1S( 0.00)
H   12       1S( 0.0)2S( 0.01)                           no 2s in beta
H   13       1S( 0.00)
H   13       1S( 0.01)2S( 0.01)                           no 2s in beta
H   14       1S( 0.01)
H   14       1S( 0.01)2S( 0.01)                            no 2s in beta
H   15       1S( 0.00)
H   15       1S( 0.0)2S( 0.01)                              no 2s in
beta
```