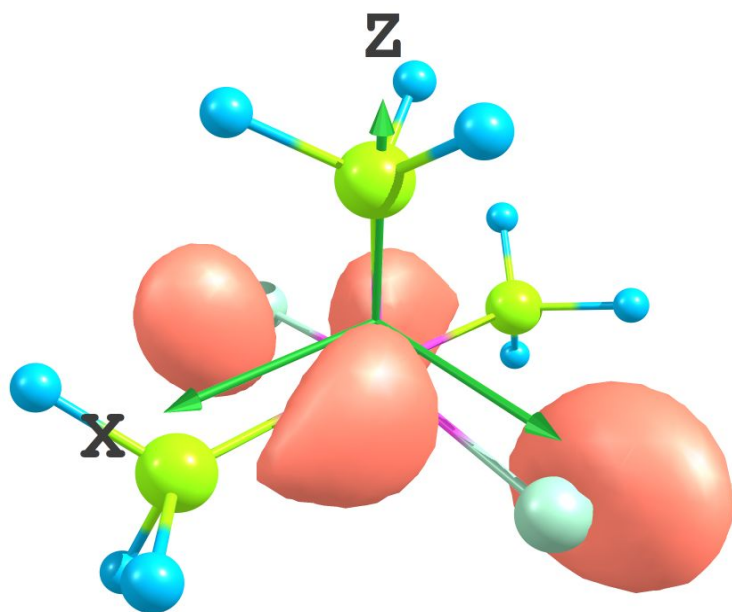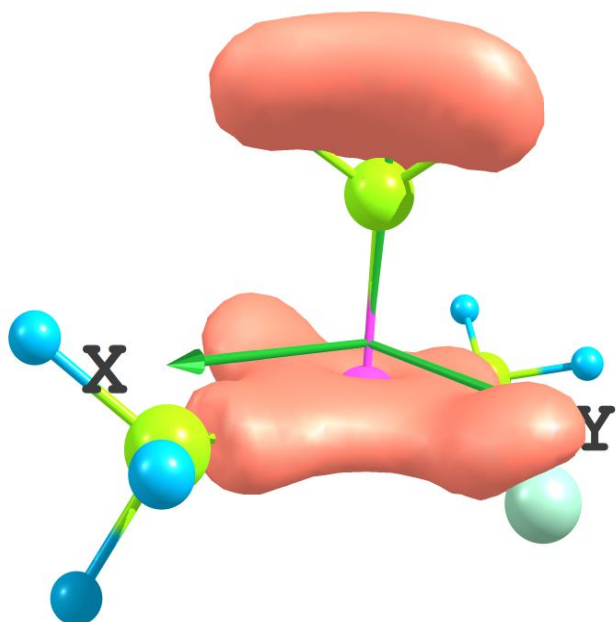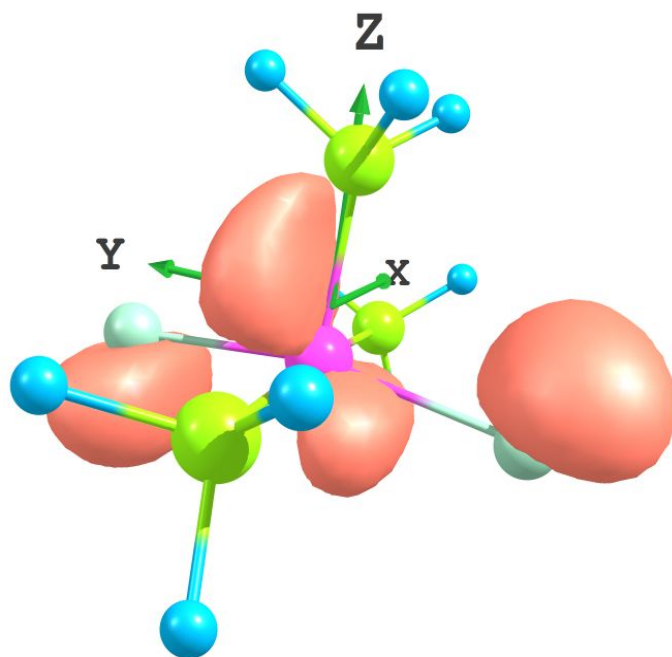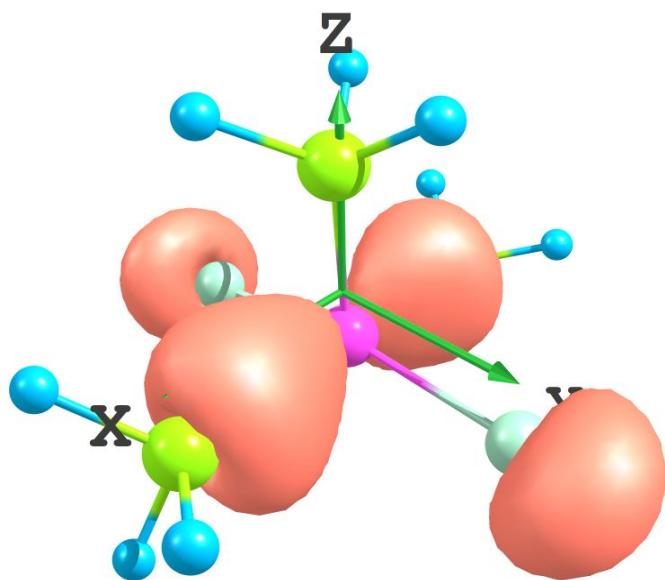In all figures, CCSD is on the left and B3LYP is on the right. In tables, CCSD is colored red and B3LYP is colored blue.

HOMO

HOMO -1

HOMO – 2

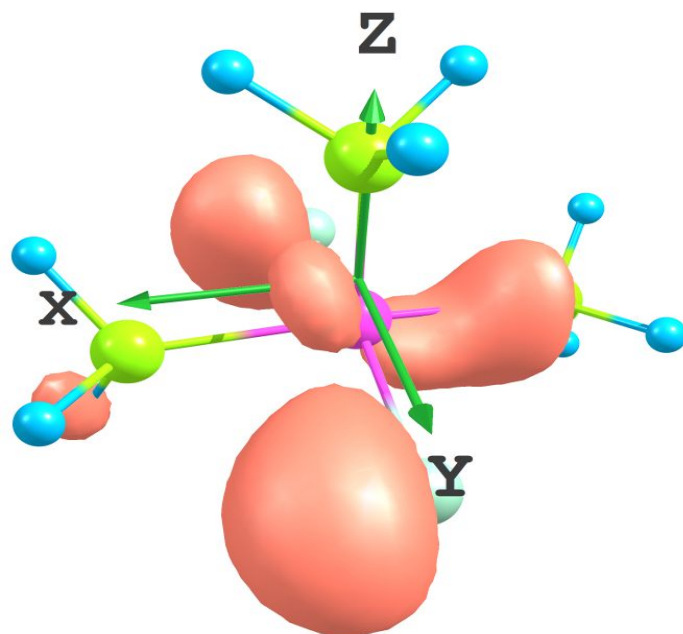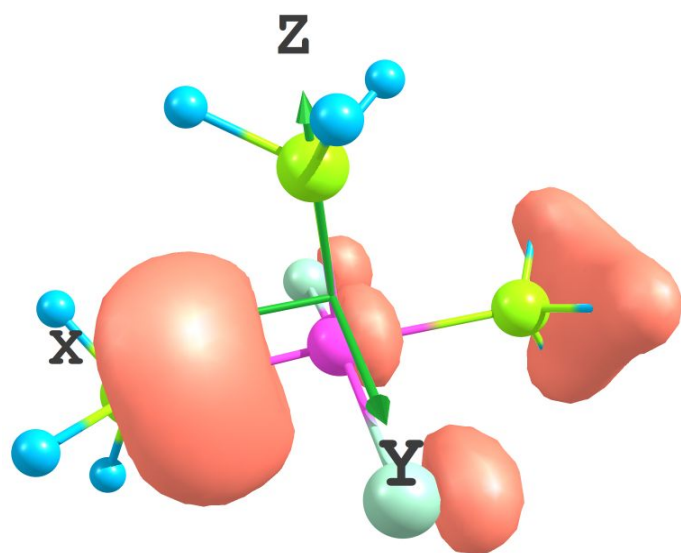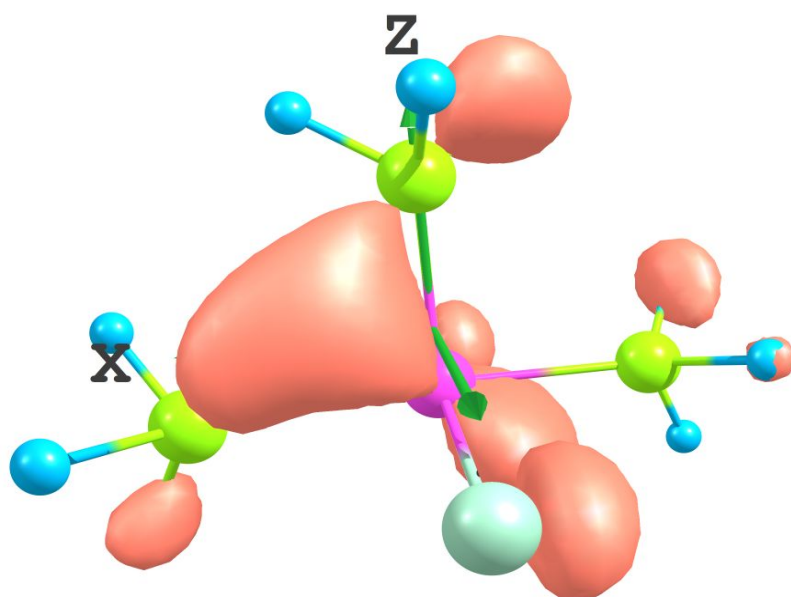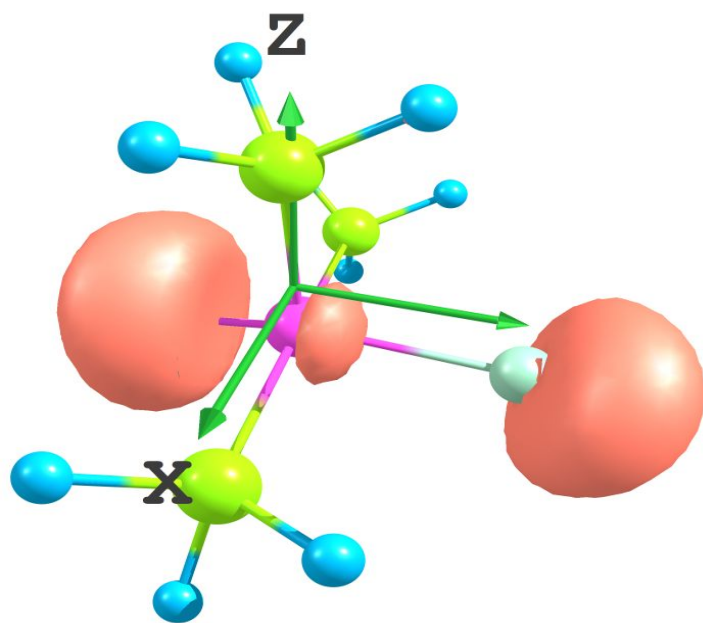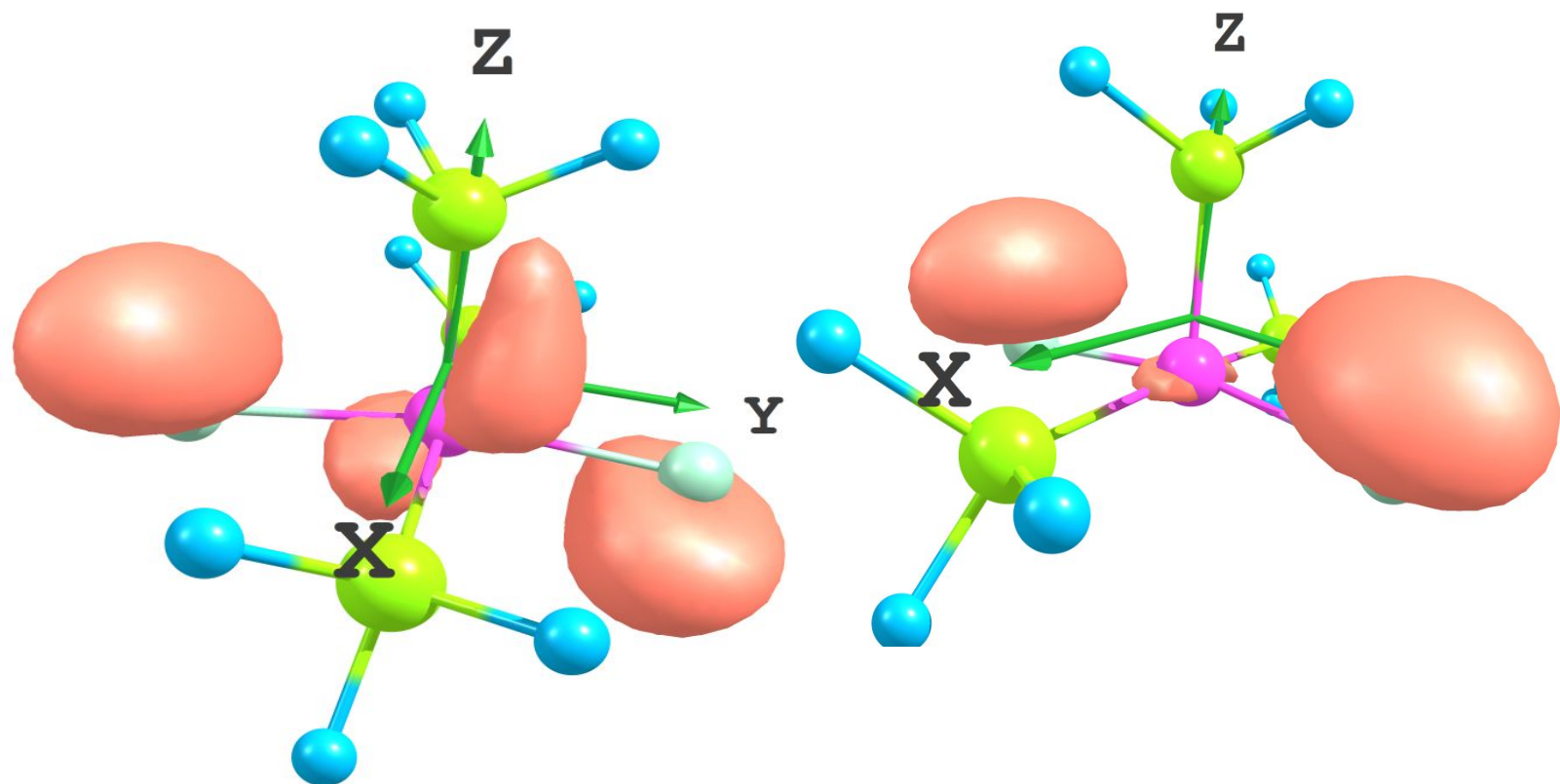HOMO – 3

HOMO – 4

LUMO
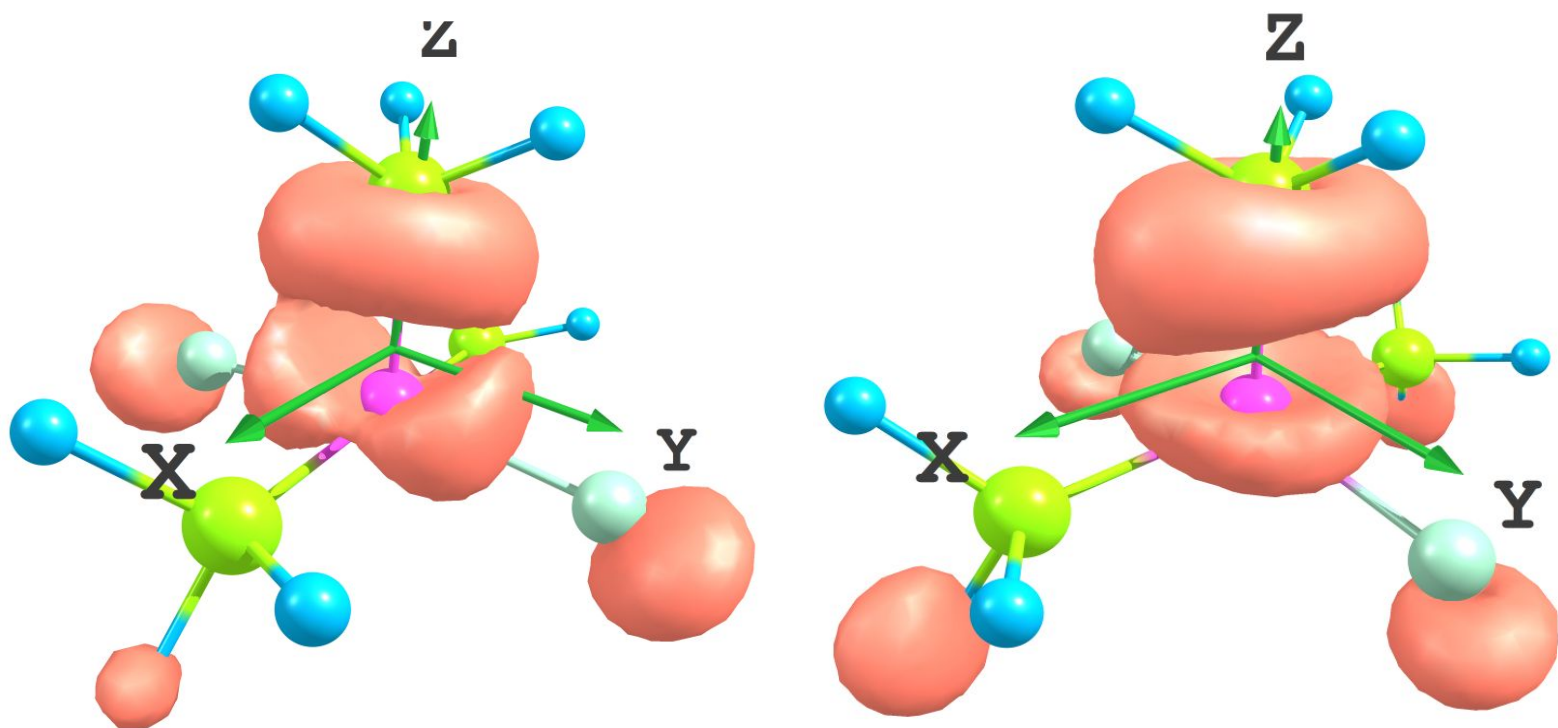
LUMO + 1
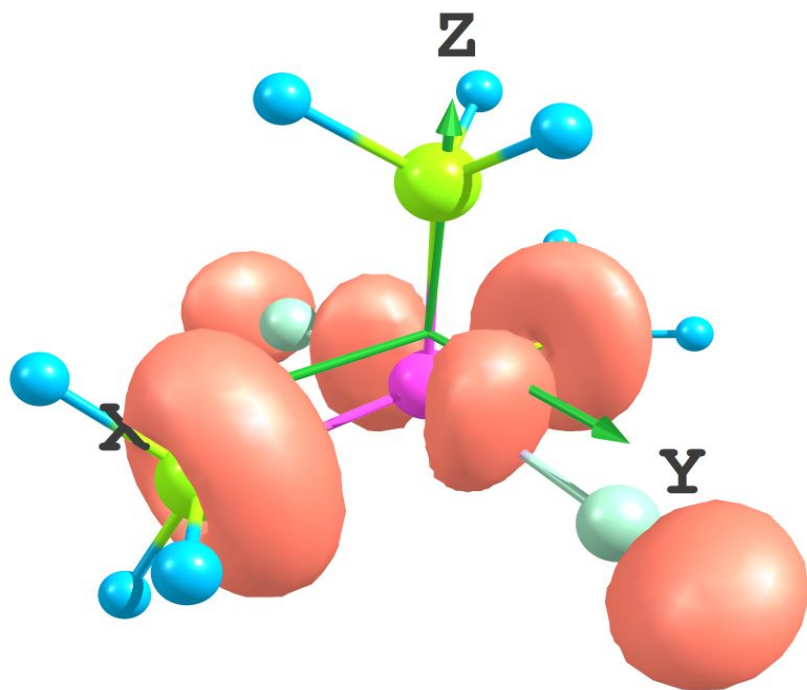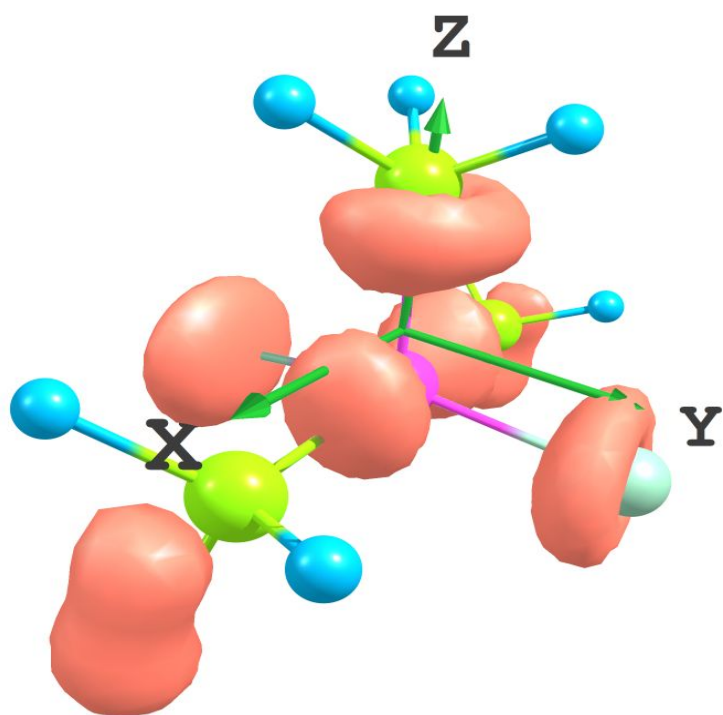
LUMO+2
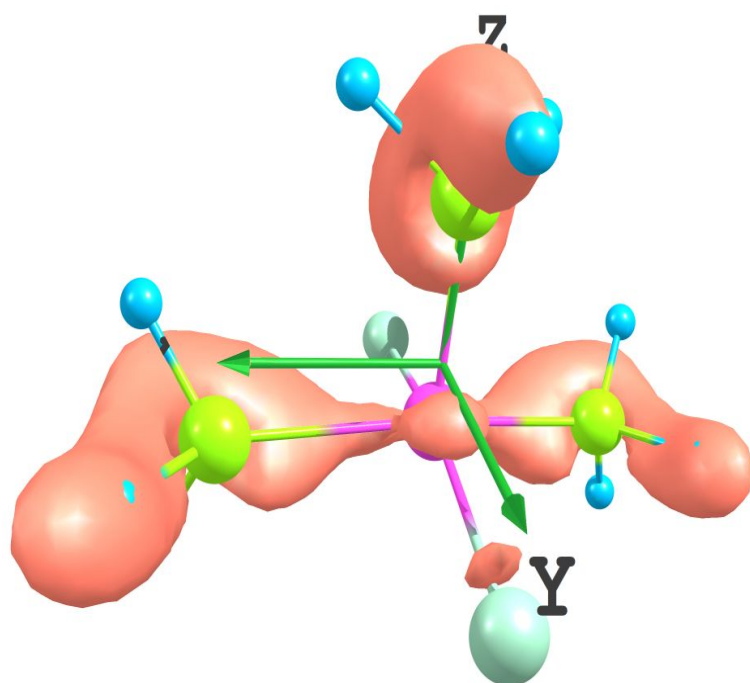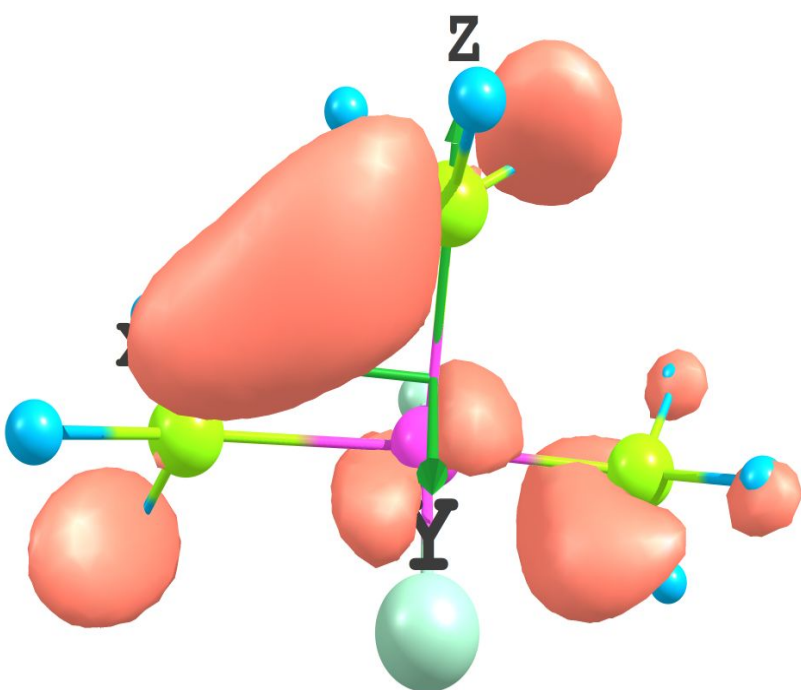
LUMO + 3
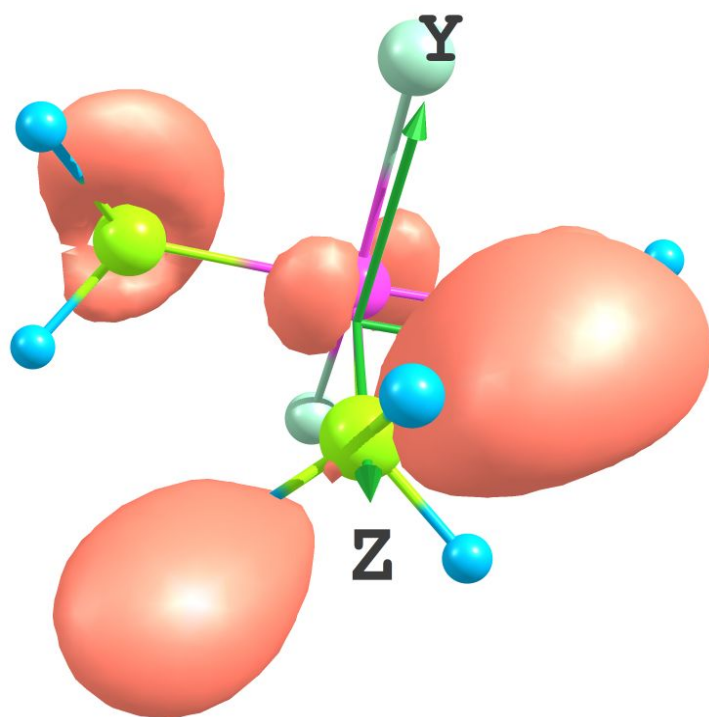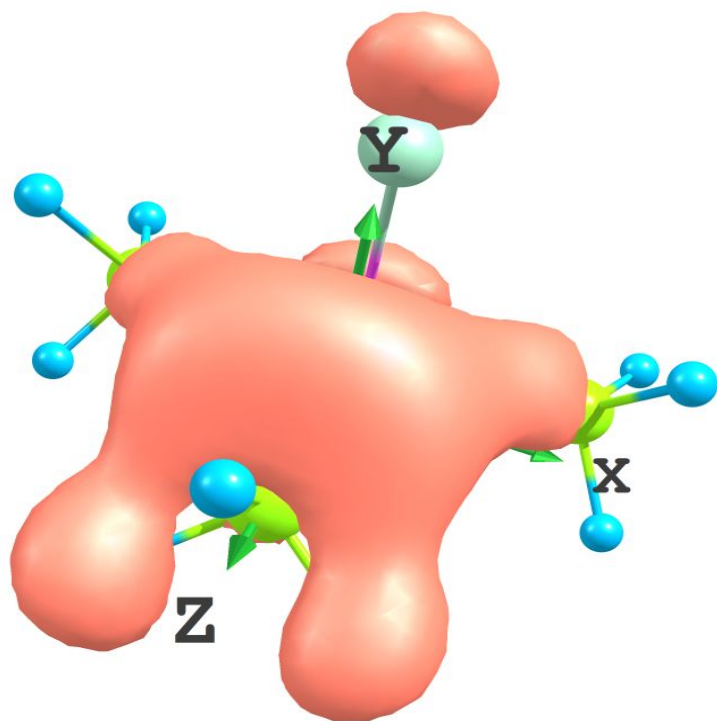
LUMO + 4
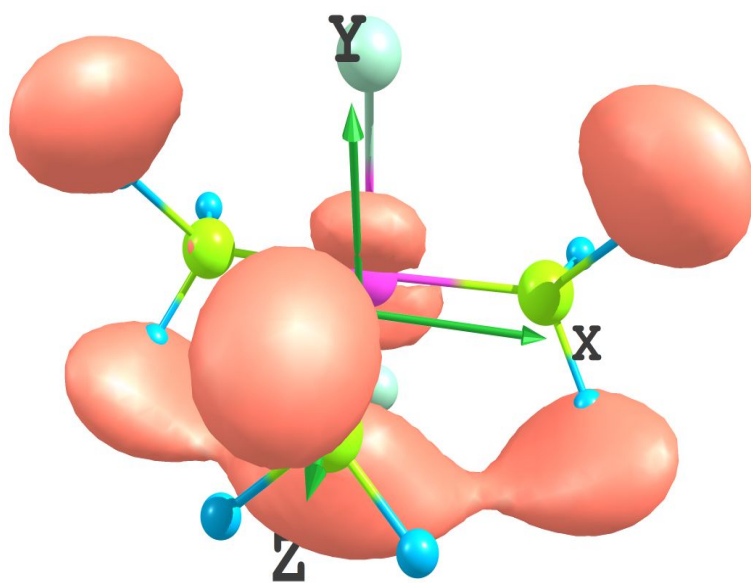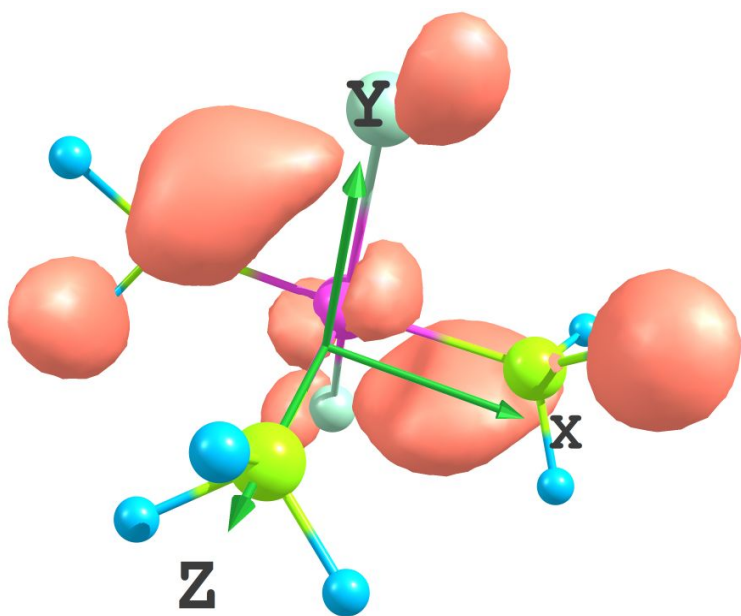
CCSD

[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)   1.99077
  7  Ru   1  px     Cor( 4p)   1.99420
 11  Ru   1  py     Cor( 4p)   1.99658
 15  Ru   1  pz     Cor( 4p)   1.98608
 79  P    3  S      Cor( 2S)   1.99729
116  P    4  S      Cor( 2S)   1.99729
190  P    6  S      Cor( 2S)   1.99607
```

B3LYP

[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)    1.99347
  7  Ru   1  px    Cor( 4p)    1.99740
 11  Ru   1  py    Cor( 4p)    1.99898
 15  Ru   1  pz    Cor( 4p)    1.98853
 79  P    3  S     Cor( 2S)    1.99783
116  P    4  S     Cor( 2S)    1.99783
190  P    6  S     Cor( 2S)    1.99674
```

Natural Population CCSD

```
Effective Core        28.00000
Core                  57.95443 ( 99.9214% of  58)
Valence               45.10758 ( 98.0600% of  46)
Natural Minimal Basis   131.06201 ( 99.2894% of 132)
Natural Rydberg Basis     0.93799 (  0.7106% of 132)
```

Natural Population B3LYP
---

```
Effective Core        28.00000
Core                  57.96764 ( 99.9442% of  58)
Valence               45.78591 ( 99.5346% of  46)
Natural Minimal Basis   131.75355 ( 99.8133% of 132)
Natural Rydberg Basis     0.24645 (  0.1867% of 132)
```

Atom No   Natural Electron Configuration. Red is CCSD and blue is B3LYP

Ru   1   [core]5S(0.42)4d(7.64)5p(0.87)4f(0.03)5d(0.07)6p(0.01)6d(0.01)
Ru   1   [core]5S(0.42)4d(7.85)5p(0.81)5d(0.02)
Cl   2   [core]3S(1.84)3p(5.40)3d(0.10)4p(0.03)4f(0.01)
Cl   2   [core]3S(1.87)3p(5.48)3d(0.01)4p(0.01)
 P   3   [core]3S(1.30)3p(3.02)3d(0.08)4p(0.02)4f(0.01)
 P   3   [core]3S(1.35)3p(3.10)3d(0.03)4p(0.01)
 P   4   [core]3S(1.30)3p(3.02)3d(0.08)4p(0.02)4f(0.01)
 P   4   [core]3S(1.35)3p(3.10)3d(0.03)4p(0.01)
Cl   5   [core]3S(1.84)3p(5.40)3d(0.10)4p(0.03)4f(0.01)
Cl   5   [core]3S(1.87)3p(5.49)3d(0.01)
 P   6   [core]3S(1.21)3p(2.87)3d(0.10)4p(0.02)4f(0.01)
 P   6   [core]3S(1.25)3p(2.96)3d(0.05)4p(0.01)

Moving to Lumo
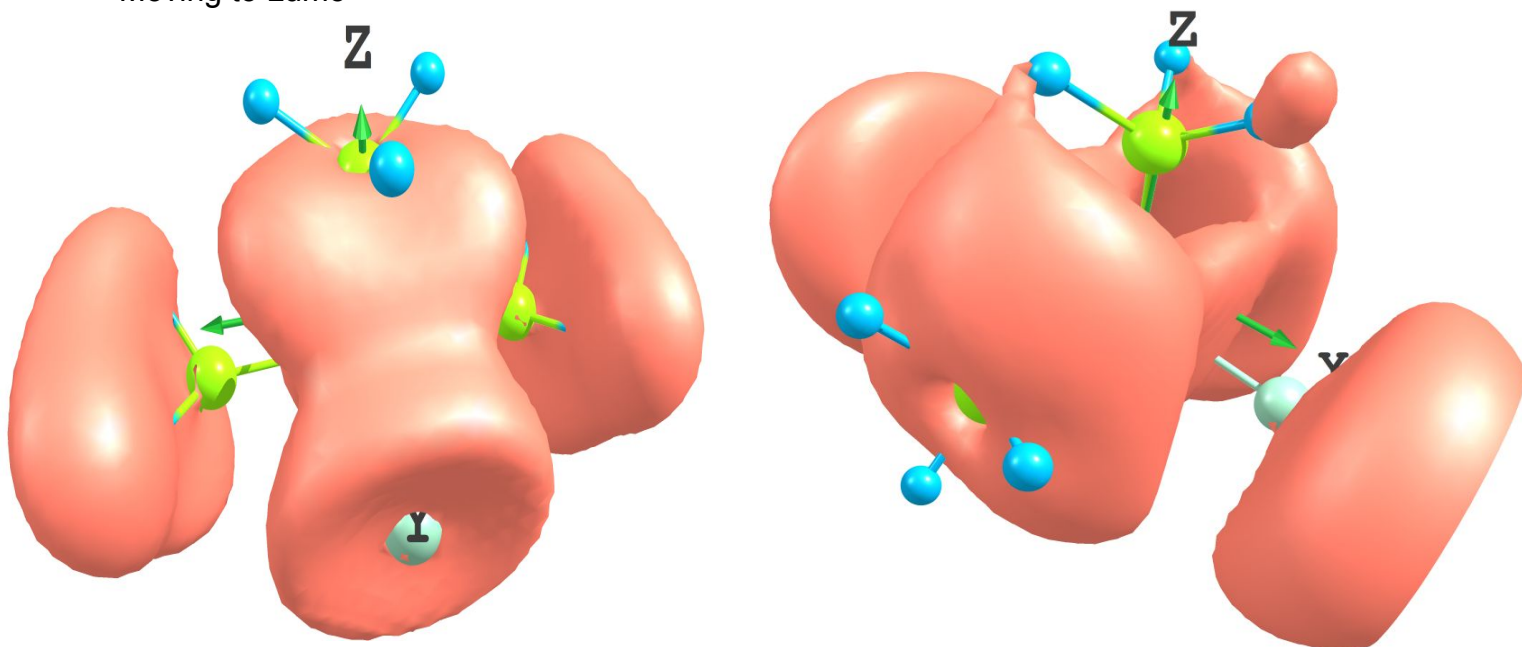
Atom No   Natural Electron Configuration

Ru   1   [core]5S(0.00)4d(0.50)5p(0.02)5d(0.00)
Ru   1   [core]5S(0.01)4d(0.39)5p(0.13)5d(0.0)
Cl   2   [core]3S(0.01)3p(0.08)4S(0.01)3d(0.01)4p(0.01) beta does not have 4s, 3d, and 4p
Cl   2   [core]3S(0.00)3p(0.04)

P   3   [core]3S(0.00)3p(0.00)3d(0.00)
P   3   [core]3S(0.01)3p(0.03)3d(0.00)4p(0.01)   beta has no 4p
P   4   [core]3S(0.00)3p(0.01)3d(0.00)
P   4   [core]3S(0.01)3p(0.03)3d(0.00)4p(0.01)   beta has no 4p
Cl   5   [core]3S(0.01)3p(0.09)4S(0.01)3d(0.01)4p(0.01)   beta does not
have 4s, 3d, and 4p
Cl   5   [core]3S(0.00)3p(0.04)3d(0.01)   beta has no 3d
P   6   [core]3S(0.07)3p(0.11)3d(0.00)
P   6   [core]3S(0.07)3p(0.11)3d(0.00)4p(0.02)   beta has no 4p
H   7   1S(0.00)
H   7   1S(0.01)
H   8   1S(0.00)
H   8   1S(0.01)
H   9   1S(0.00)
H   9   1S(0.01)
H 10   1S(0.00)
H 10   1S(0.01)
H 11   1S(0.00)
H 11   1S(0.00)
H 12   1S(0.00)
H 12   1S(0.02)
H 13   1S(0.00)
H 13   1S(0.02)
H 14   1S(0.01)
H 14   1S(0.00)
H 15   1S(0.01)
H 15   1S(0.01)

Moving to Lumo+1
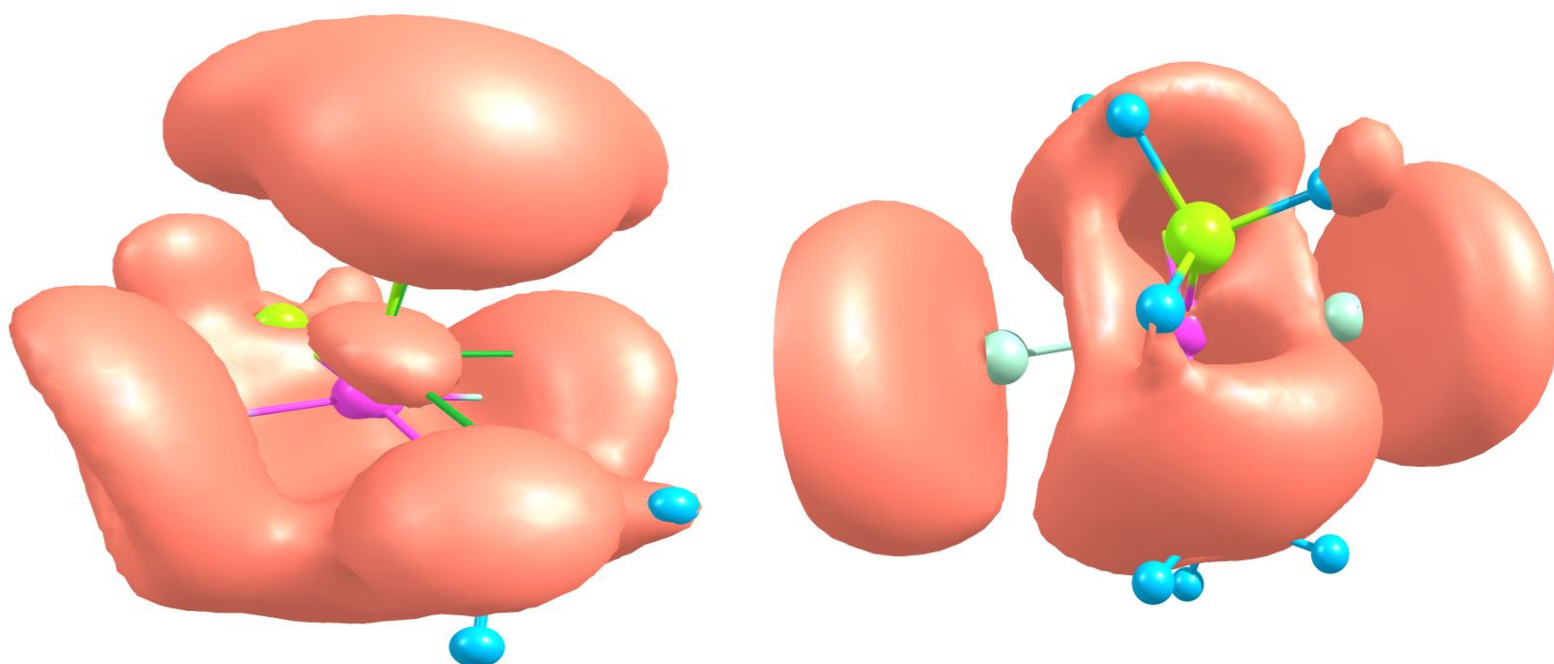
```
      Atom  No         Natural Electron Configuration
  -----------------------------------------------------------------------

    Ru    1     [core]5S( 0.01)4d( 0.44)5p( 0.01)6S( 0.01)5d( 0.00)          beta has no
6s
    Ru    1     [core]5S( 0.00)4d( 0.59)5p( 0.00)5d( 0.00)
    Cl    2     [core]3S( 0.01)3p( 0.05)3d( 0.01)4p( 0.01)          beta has no 3d and
4p
    Cl    2     [core]3S( 0.02)3p( 0.10)3d( 0.01)                    beta does not
have 3d
    P    3     [core]3S( 0.06)3p( 0.09)3d( 0.00)
    P    3     [core]3S( 0.06)3p( 0.06)3d( 0.01)4p( 0.03)          beta does not have
4p
    P    4     [core]3S( 0.06)3p( 0.09)3d( 0.00)
    P    4     [core]3S( 0.06)3p( 0.06)3d( 0.01)4p( 0.03)           beta does not
have 4p
    Cl    5     [core]3S( 0.01)3p( 0.06)3d( 0.01)4p( 0.01)          beta has no 3d and
4p
    Cl    5     [core]3S( 0.01)3p( 0.09)3d( 0.01)                    beta does not
have 3d
    P    6     [core]3S( 0.02)3p( 0.04)3d( 0.00)
    P    6     [core]3S( 0.00)3p( 0.00)3d( 0.00)
    H    7         1S( 0.00)
    H    7         1S( 0.00)
    H    8         1S( 0.00)
    H    8         1S( 0.00)
    H    9         1S( 0.00)
    H    9         1S( 0.00)
    H   10         1S( 0.00)
    H   10         1S( 0.01)
    H   11         1S( 0.00)
    H   11         1S( 0.01)
    H   12         1S( 0.00)
    H   12         1S( 0.00)
    H   13         1S( 0.00)
    H   13         1S( 0.00)
    H   14         1S( 0.00)
    H   14         1S( 0.01)
    H   15         1S( 0.00)
    H   15         1S( 0.01)
```