



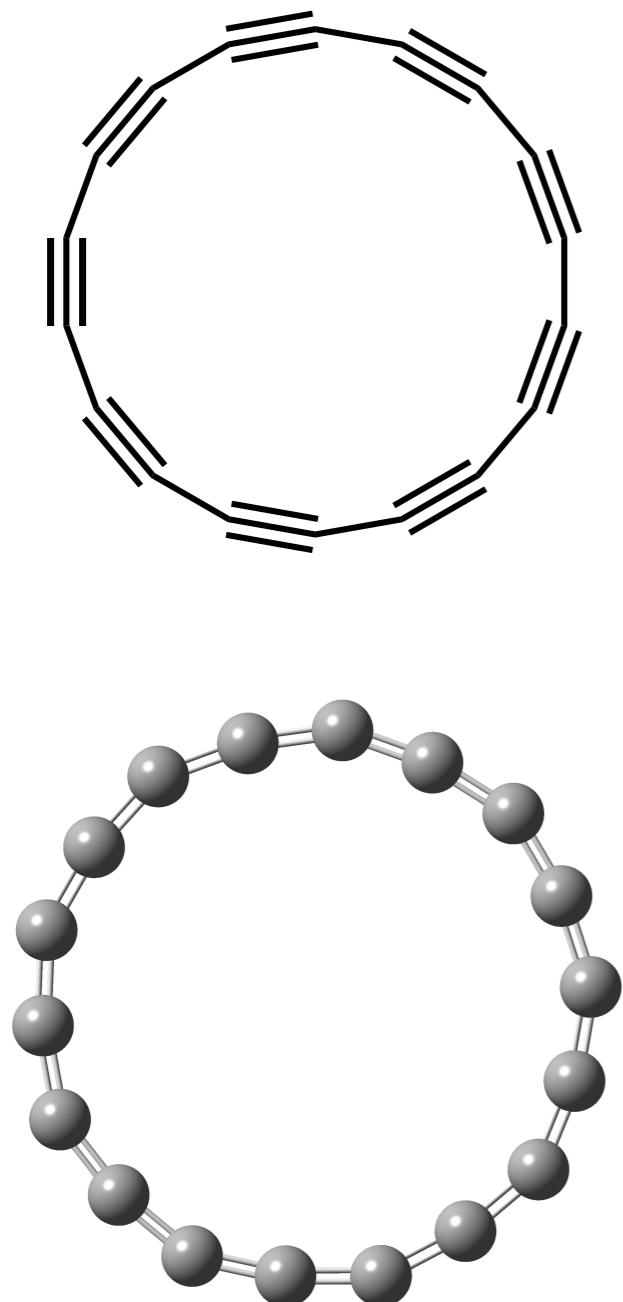
HIROSHIMA UNIVERSITY

# AICD Analysis of Cyclo[18]carbon

- Geometry Optimization ..... 1
- AICD Analysis with all molecular orbitals ..... 2
- AICD Analysis with  $\pi$  orbitals ..... 5

# Geometry Optimization

## [ Structure ]



## [ Optimization Input ]

```
%nprocshared=6  
%mem=6GB  
%chk=c18_opt.chk  
#p opt freq rb3lyp/6-31g(d)
```

Title Card Required

| 0 | 1 |             |             |
|---|---|-------------|-------------|
| C |   | -0.01100000 | 2.58500000  |
| C |   | -0.01600000 | 3.28600000  |
| C |   | -0.01900000 | 3.65900000  |
| C |   | -0.01900000 | 3.56900000  |
| C |   | -0.01600000 | 3.00200000  |
| C |   | -0.01100000 | 2.16400000  |
| C |   | 0.01100000  | -1.08900000 |
| C |   | 0.01800000  | -2.17100000 |
| C |   | 0.02300000  | -3.13400000 |
| C |   | 0.02600000  | -3.62700000 |
| C |   | 0.02600000  | -3.73000000 |
| C |   | 0.02300000  | -3.40500000 |
| C |   | 0.01800000  | -2.60100000 |
| C |   | 0.01100000  | -1.60900000 |
| C |   | 0.00300000  | 0.28300000  |
| C |   | -0.00400000 | 1.44600000  |
| C |   | 0.00300000  | -0.27300000 |
| C |   | -0.00400000 | 0.92200000  |

# AICD Analysis >> All MOs

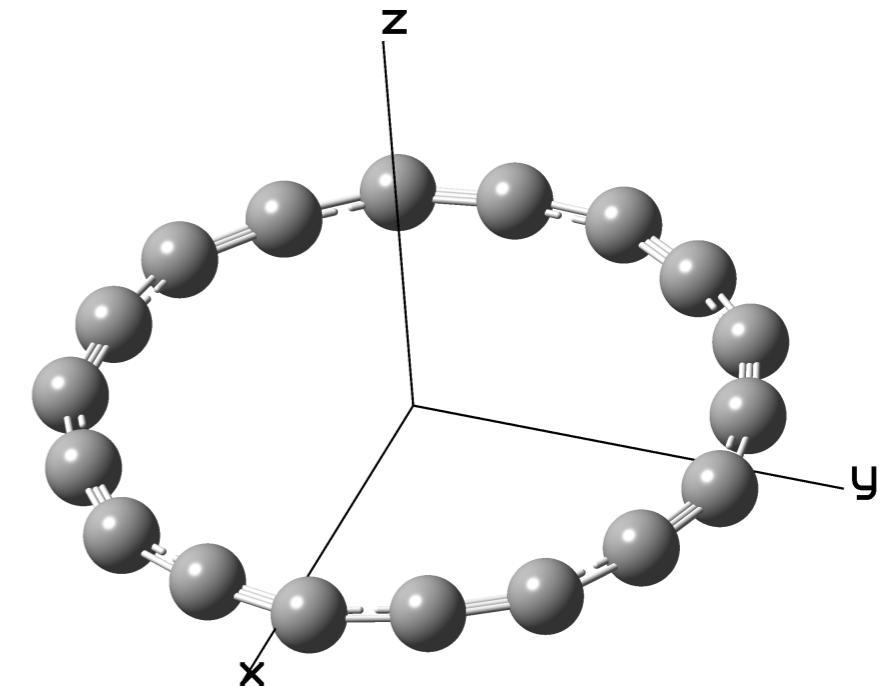
## [ Input ]

```
%nprocshared=6  
%mem=10GB  
%chk=c18_nmr_all.chk  
#p nmr=csgt rb3lyp/6-31g(d) iop(10/93=1)
```

Title Card Required

| 0 | 1           |             |             |
|---|-------------|-------------|-------------|
| C | 3.50887638  | -1.00354618 | -0.00003053 |
| C | 3.72695833  | 0.26291456  | -0.00003578 |
| C | 3.33313822  | 1.48654723  | 0.00003099  |
| C | 2.68571049  | 2.59661085  | 0.00003931  |
| C | 1.59752514  | 3.28092840  | -0.00003077 |
| C | 0.38804451  | 3.71504122  | -0.00003851 |
| C | 0.90613627  | -3.62391161 | 0.00001936  |
| C | -0.37897022 | -3.62896224 | -0.00000209 |
| C | -1.63547496 | -3.35853724 | -0.00002503 |
| C | -2.62346512 | -2.53665578 | -0.00003439 |
| C | -3.41213853 | -1.52169797 | -0.00001772 |
| C | -3.64072294 | -0.25704648 | 0.00001830  |
| C | -3.59193276 | 1.02739476  | 0.00002180  |
| C | -2.95406946 | 2.14301102  | 0.00000514  |
| C | 2.04261652  | -3.02367017 | 0.00005359  |
| C | 3.02393013  | -2.19388991 | 0.00000085  |
| C | -2.09090348 | 3.09539100  | 0.00003618  |
| C | -0.88525852 | 3.54007852  | -0.00001070 |

c18\_nmr\_all.txt



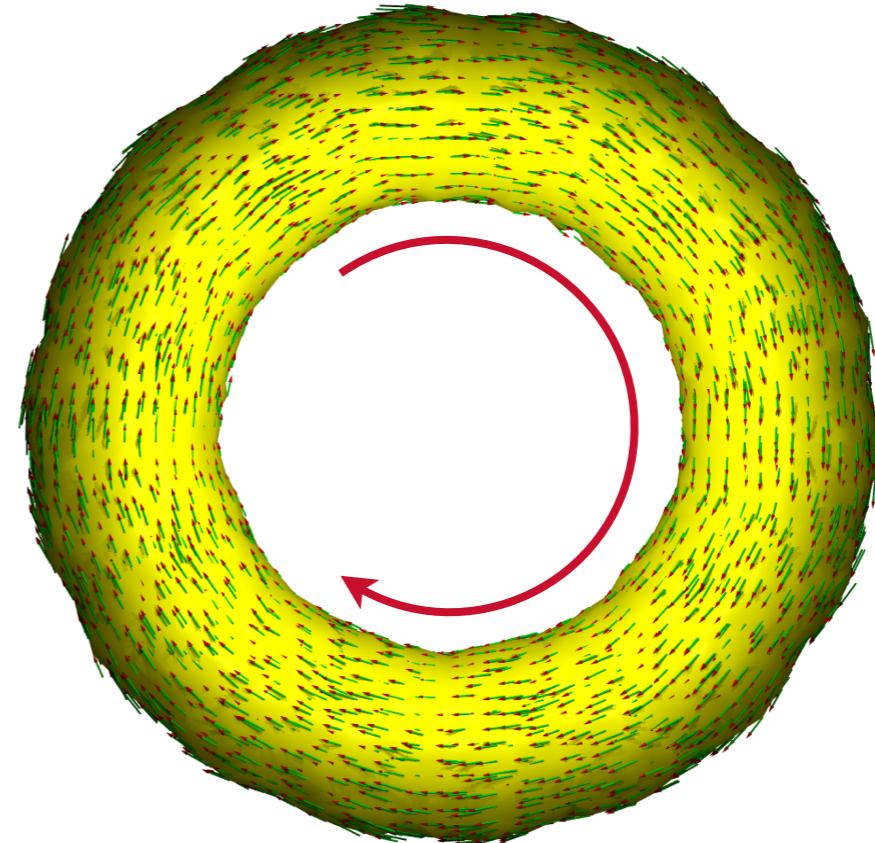
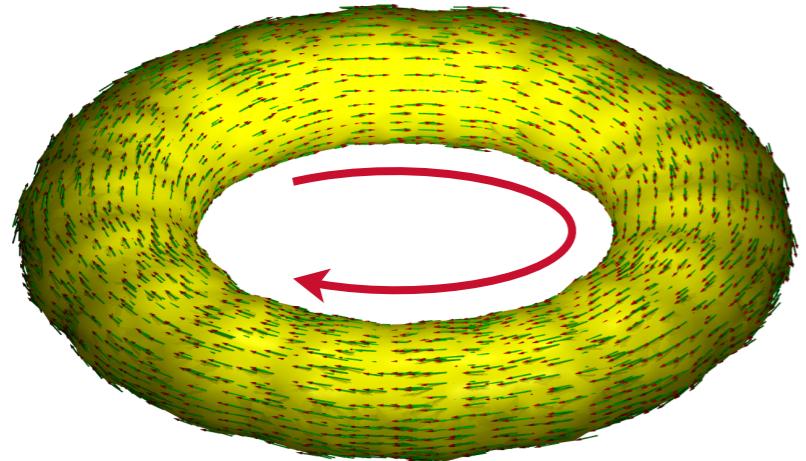
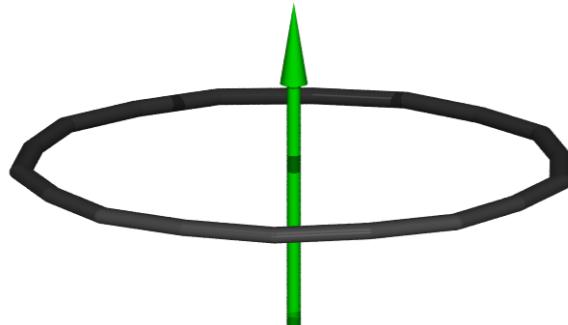
# AICD Analysis >> All MOs

## [ AICD Analysis ]

```
AICD -m 2 -p 60000 -b 0 0 1 --maxarrowlength 1 -s --povrayinput -c c18_nmr_all.log
```

60000 data points  
omit arrows  
longer than 1  
Singlet view  
with arrows  
external magnetic  
field along z axis  
smoother  
.out file name

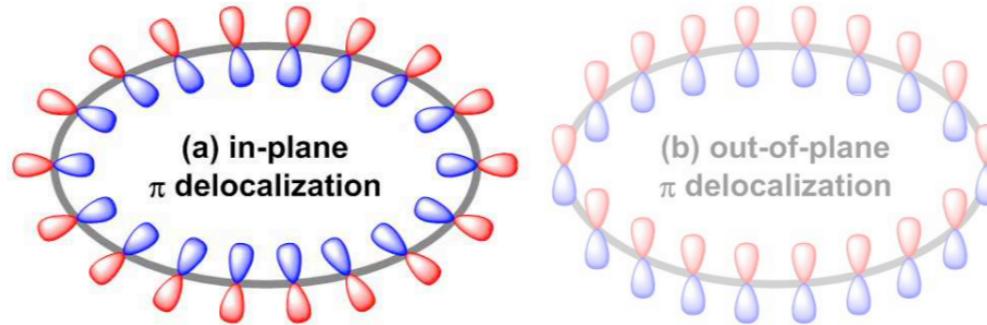
$B_0$



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# AICD Analysis >> In-plane $\pi$ Orbitals

## [ $\pi$ Electron Delocalizations in the Cyclo[18]carbon ]



### [ Input ]

```
%nprocshared=6  
%mem=10GB  
%chk=c18_nmr_in.chk  
#p nmr=csgt rb3lyp/6-31g(d) iop(10/93=2)
```

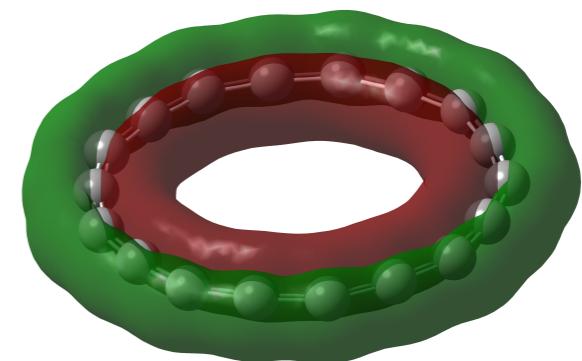
Z. Liu, T. Lu, Q. Chen, *Carbon*, 165 (2020), 468-475.

Title Card Required

```
0 1  
C           3.50887638   -1.00354618   -0.00003053  
.....  
C          -0.88525852    3.54007852   -0.00001070
```

c18\_nmr\_in.txt

```
37  
39  
40  
45  
46  
49  
50  
53  
54
```



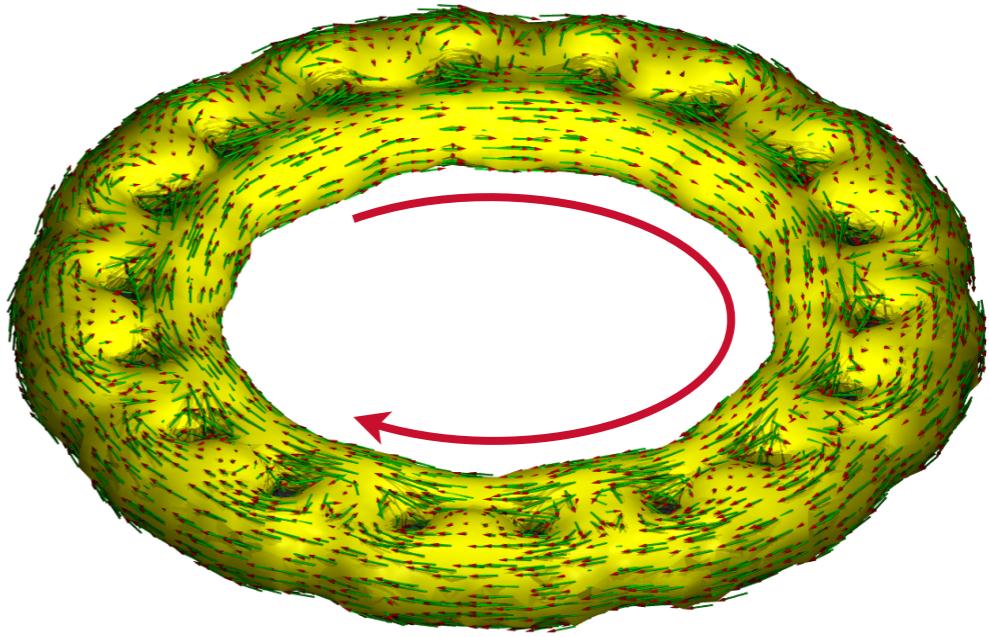
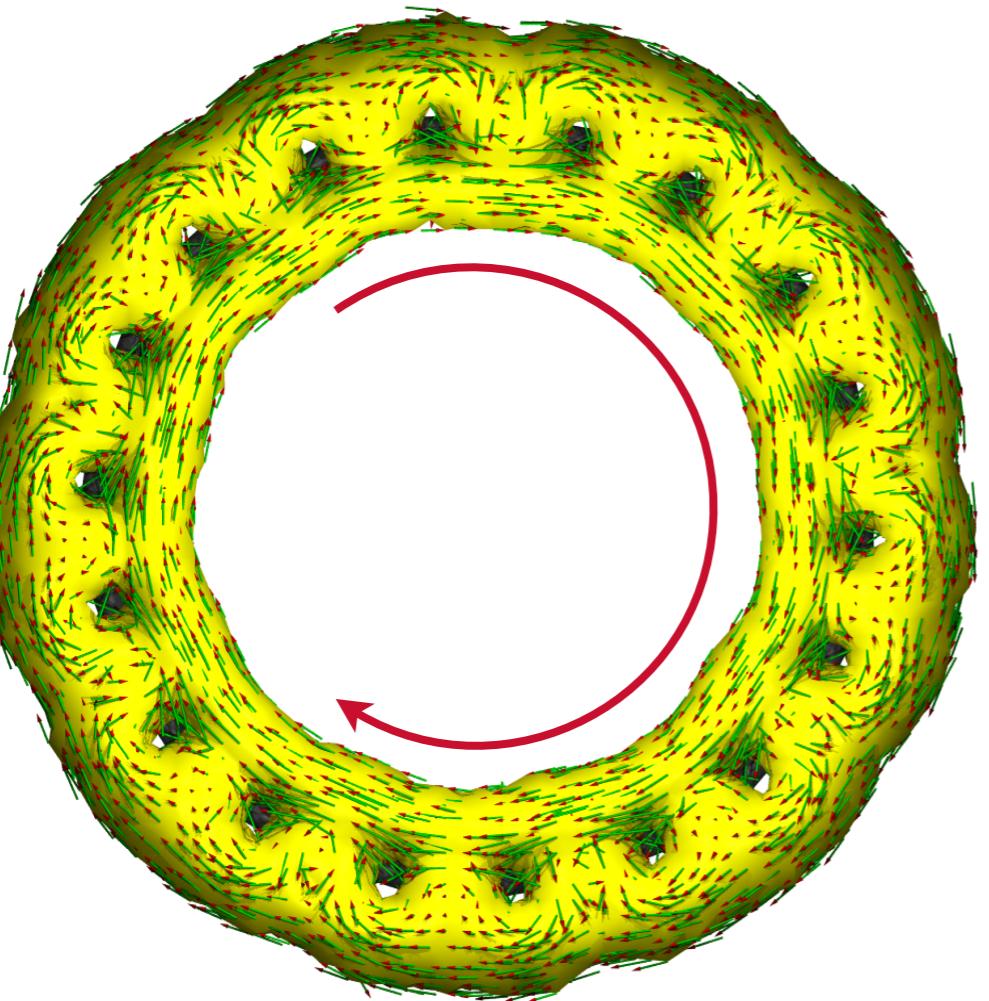
MO = 37

# AICD Analysis >> In-plane $\pi$ Orbitals

## [ AICD Analysis ]

```
AICD -m 2 -p 60000 -b 0 0 1 -1 0.07 -s -povrayinput -c c18_nmr_in.log
```

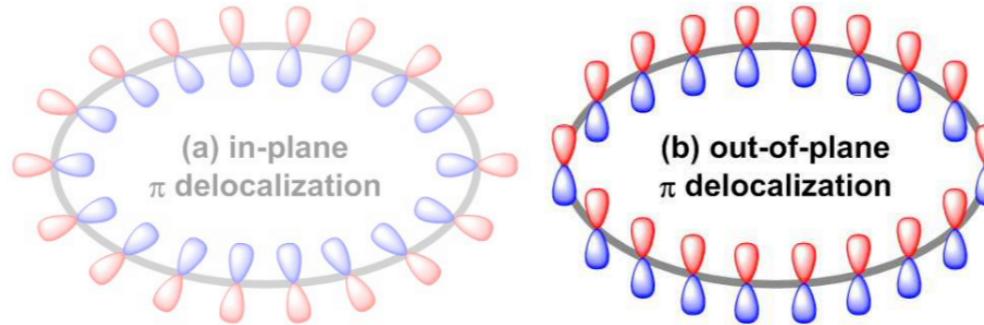
isovalue = 0.07



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# AICD Analysis >> Out-of-plane $\pi$ Orbitals

## [ $\pi$ Electron Delocalizations in the Cyclo[18]carbon ]



### [ Input ]

```
%nprocshared=6  
%mem=10GB  
%chk=c18_nmr_out.chk  
#p nmr=csgt rb3lyp/6-31g(d) iop(10/93=2)
```

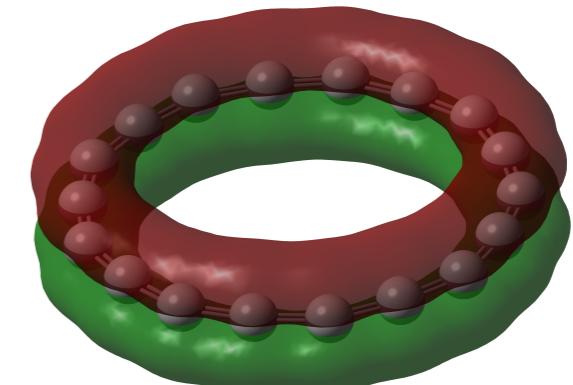
Z. Liu, T. Lu, Q. Chen, *Carbon*, 165 (2020), 468-475.

Title Card Required

```
0 1  
C           3.50887638   -1.00354618   -0.00003053  
.....  
C          -0.88525852    3.54007852   -0.00001070
```

c18\_nmr\_out.txt

```
38  
41  
42  
43  
44  
47  
48  
51  
52
```

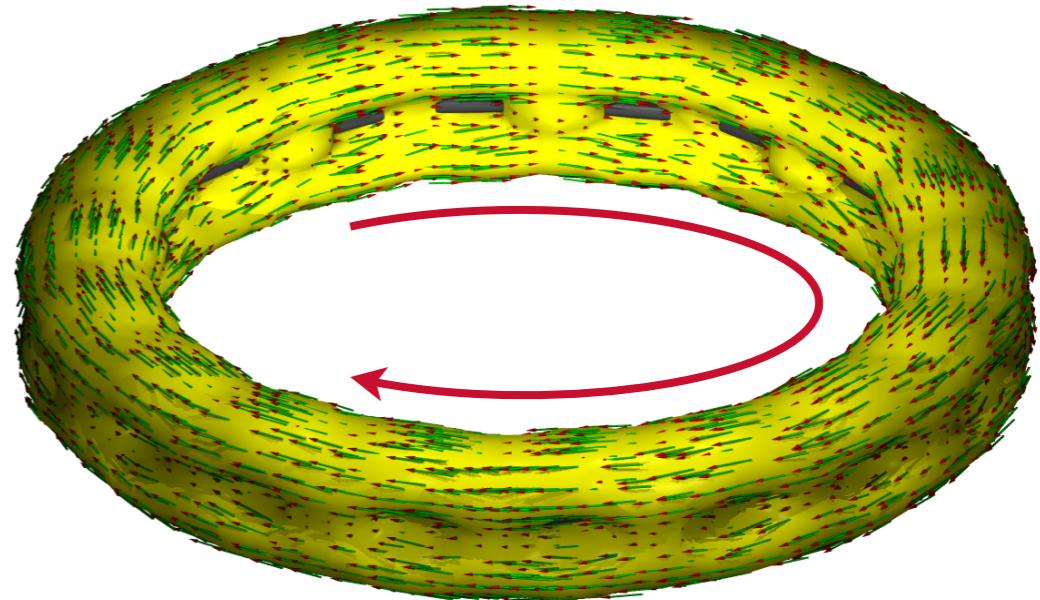
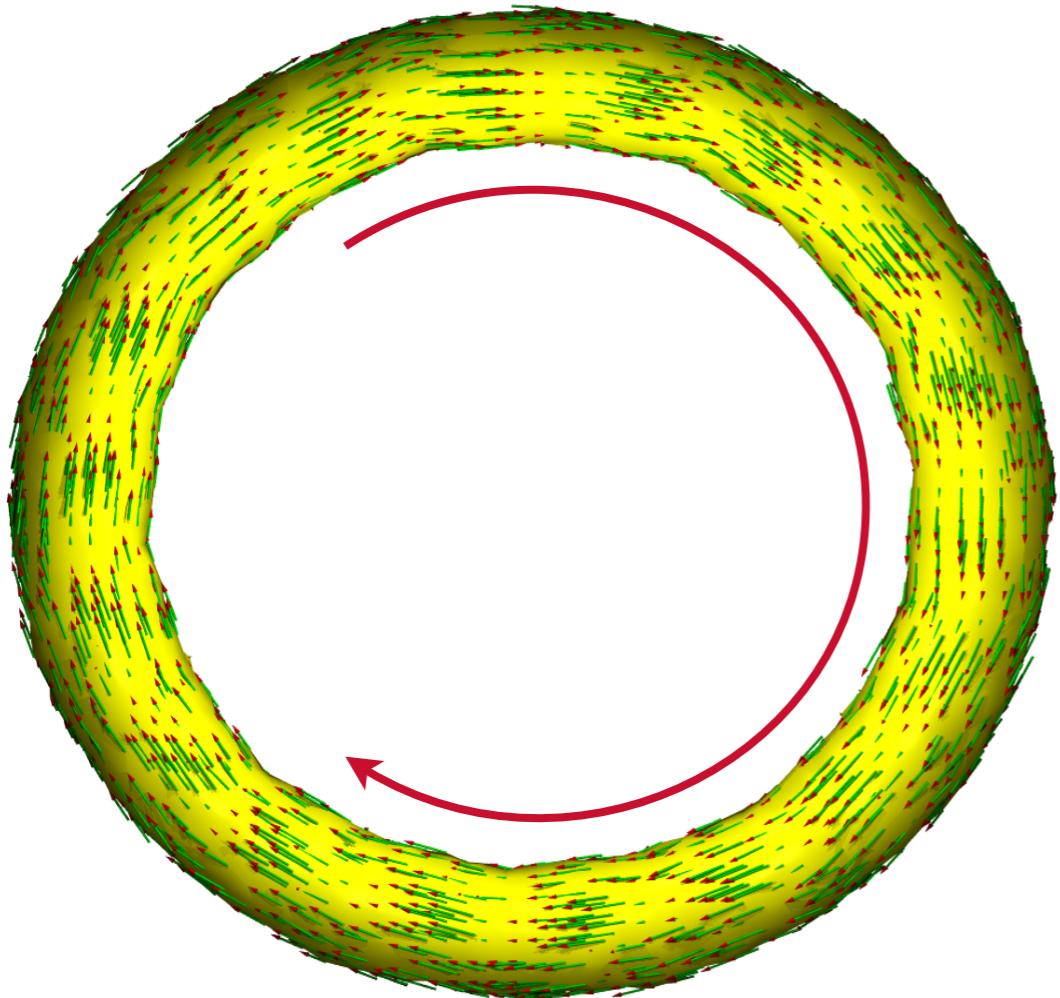


MO = 38

# AICD Analysis >> Out-of-plane $\pi$ Orbitals

## [ AICD Analysis ]

```
AICD -m 2 -p 60000 -b 0 0 1 -l 0.07 -s --povrayinput -c c18_nmr_out.log
```



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