Coordinates, onsite energies and hopping matrices

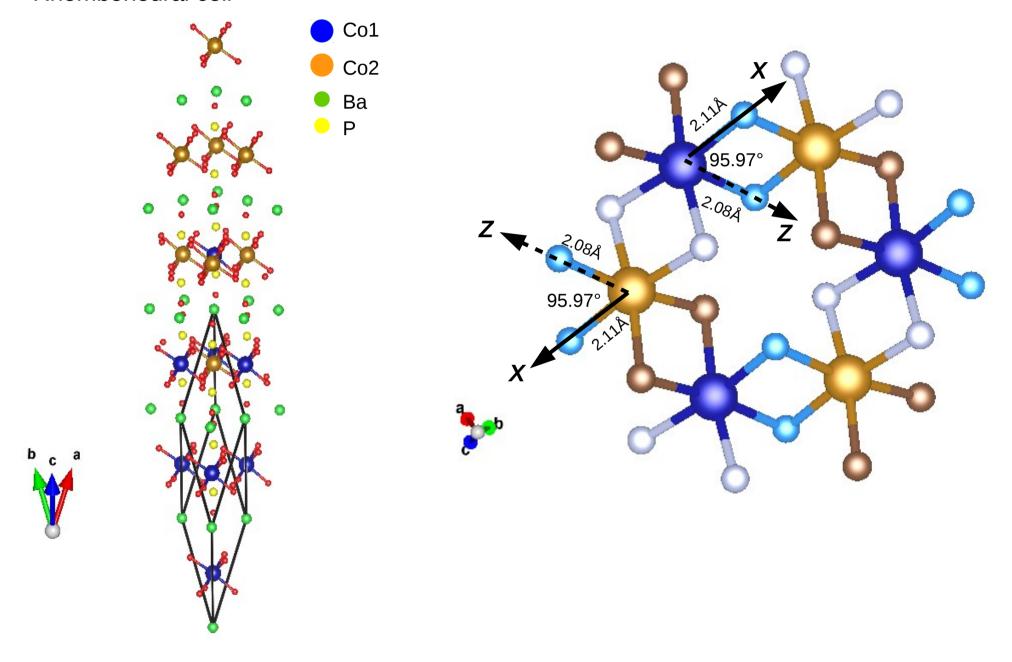
BaCo₂(PO₄)₂

9.2.2021

Coordinate_BaCo₂(PO₄)₂

Space group: *R-3* (148)

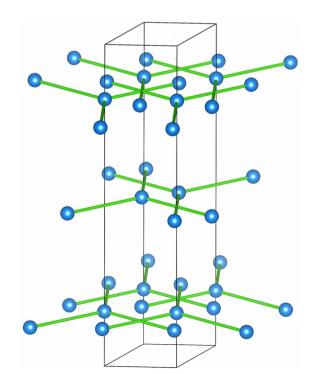
Rhombohedral cell



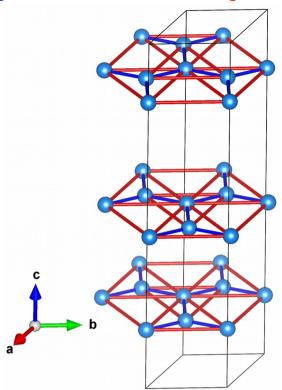
BaCo₂(PO₄)₂ Co-Co neighbors

Co-Co Bond-length (Å)	Numbers
2.8081	3
4.8554	6
5.6090	3
7.4186	6

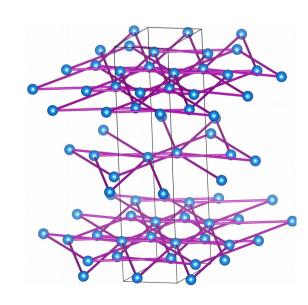
5.6090Å



Nearest neighbor & next nearest neighbor



7.4186Å



Onsite energies eV

Co₁

	dxy	dyz	d3z^2-1	dxz	dx^2-y^2
dxy	-3.4155	0.0008	0.0157	0.0017	-0.0900
dyz	0.0008	-3.5049	0.0008	-0.0717	0.0034
d3z^2-1	0.0157	8000.0	-3.1860	0.0249	0.5051
dxz	0.0017	-0.0717	0.0249	-2.2912	-0.0136
dx^2-y^2	-0.0900	0.0034	0.5051	-0.0136	-2.5757

Co₂

	dxy	dyz	d3z^2-1	dxz	dx^2-y^2
dxy	-3.4155	-0.0008	-0.0157	0.0017	0.0900
dyz	-0.0008	-3.5049	0.0008	0.0717	0.0034
d3z^2-1	-0.0157	8000.0	-3.1860	-0.0249	0.5051
dxz	0.0017	0.0717	-0.0249	-2.2912	0.0136
dx^2-y^2	0.0900	0.0034	0.5051	0.0136	-2.5757

3-6-4.out rotation

Co2-Co1 & Co1-Co2 hopping matrices (H1) eV unit

Co-Co Bond length: 2.8081 (Å) Numbers: 3 Hopping matrix: H1

Co2-Co1

Co1-Co2

Int.bet. Co1- 3/Co1- 2 Dist=1.0017 Trans. vecs. : 0 0 1 Connecting vector: -0.500-0.866-0.059								
-	dxy	dyz	d3z^2-1	dxz	dx^2-y^2			
dxy	-0.0363	0.0024	0.0519	-0.0106	0.0057			
dyz	-0.0024	0.1162	0.0031	0.0458	-0.0152			
d3z^2-1	-0.0519	0.0031	-0.2813	0.0216	0.1553			
dxz	-0.0106	-0.0458	-0.0217	0.0748	0.0078			
dx^2-y^2	-0.0057	-0.0152	0.1553	-0.0078	-0.1642			

Int.bet. Co1- 2/Co1- 3 Dist=1.0017 Trans. vecs. : 0 0-1 Connecting vector: 0.500 0.866 0.059						
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2	
dxy	-0.0363	-0.0024	-0.0519	-0.0106	-0.0057	
dyz	0.0024	0.1162	0.0031	-0.0458	-0.0152	
d3z^2-1	0.0519	0.0031	-0.2813	-0.0217	0.1553	
dxz	-0.0106	0.0458	0.0216	0.0748	-0.0078	
dx^2-y^2	0.0057	-0.0152	0.1553	0.0078	-0.1642	

Int.bet. Co1- 3/Co1- 2 Dist=1.0017 Trans. vecs. : 0 1 0 Connecting vector: -0.500 0.866-0.059							
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2		
dxy	0.1217	0.2215	0.0096	0.0265	-0.0213		
dyz	-0.2215	-0.1827	-0.0315	0.0309	0.0908		
d3z^2-1	-0.0096	-0.0315	0.0161	-0.0059	-0.0761		
dxz	0.0265	-0.0309	0.0059	0.0711	0.0043		
dx^2-y^2	0.0213	0.0908	-0.0761	-0.0043	-0.0084		

Int.bet. Co	Int.bet. Co1- 2/Co1- 3							
Dist=1.00	Dist=1.0017 Trans. vecs. : 0-1 0							
Connecting vector: 0.500-0.866 0.059								
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2			
dxy	0.1217	-0.2215	-0.0096	0.0265	0.0213			
dyz	0.2215	-0.1827	-0.0315	-0.0309	0.0908			
d3z^2-1	0.0096	-0.0315	0.0161	0.0059	-0.0761			
dxz	0.0265	0.0309	-0.0059	0.0711	-0.0043			
dx^2-y^2	-0.0213	0.0908	-0.0761	0.0043	-0.0084			

```
Int.bet. Co1- 3/Co1- 2
| IDist=1.0017 Trans. vecs. : 1 0 0
|Connecting vector: 1.000 0.000-0.059
                    dyz
                              d3z^2-1
                                                 dx^2-y^2
           dxy
                                        dxz
          0.0987
                    -0.2255
                                                  0.0137
dxy
                              0.0194
                                        -0.0309
                   -0.2091
                                        -0.0040
                                                  -0.0496
          0.2255
                              0.0435
dvz
d3z^2-1
                              -0.0103
                                        0.0031
                                                  -0.0874
          -0.0194
                    0.0435
          -0.0309
                     0.0040
                              -0.0031
                                         0.0612
                                                   0.0033
dxz
dx^2-v^2
          -0.0137
                     -0.0496
                               -0.0874
                                         -0.0033
                                                   0.0115
```

```
Int.bet. Co1- 2/Co1- 3
|Dist=1.0017 Trans. vecs. :-1 0 0
|Connecting vector: -1.000 0.000 0.059
           dxy
                     dvz
                             d3z^2-1
                                        dxz
                                                dx^2-v^2
          0.0987
                    0.2255
                                                  -0.0137
dxv
                              -0.0194
                                        -0.0309
          -0.2255
                    -0.2091
                              0.0435
                                        0.0040
                                                  -0.0496
dvz
d3z^2-1
          0.0194
                    0.0435
                              -0.0103
                                        -0.0031
                                                  -0.0874
          -0.0309
                    -0.0040
                               0.0031
                                         0.0612
                                                  -0.0033
dxz
dx^2-y^2 0.0137
                    -0.0496
                              -0.0874
                                        0.0033
                                                  0.0115
```

3-6-4.out_rotation

Co1-Co1 & Co2-Co2 hopping matrices (H2) eV unit Co-Co Bond length: 4.8554 (Å) Numbers: 6 Hopping matrix: H2

Co1-Co1

Dist=1.7321 Trans. vecs. :-1 0 1 Connecting vector: -1.500-0.866 0.000							
•	dxy	dyz	d3z^2-1	dxz	dx^2-y^2		
dxy	0.0021	-0.0101	-0.0299	-0.0016	0.0036		
dyz	0.0030	0.0008	-0.0160	0.0247	0.0185		
d3z^2-1	0.0157	0.0142	-0.0085	-0.0115	-0.0233		
dxz	-0.0313	0.0173	0.0064	-0.0005	0.0055		
dx^2-y^2	-0.0081	0.0183	0.0086	-0.0310	-0.0048		

```
|Dist=1.7321 Trans. vecs. :-1 1 0
|Connecting vector: -1.500 0.866 0.000
           dxy
                   dyz
                              d3z^2-1
                                         dxz
                                                  dx^2-y^2
          -0.0114
                    0.0220
                              -0.0084
                                         0.0191
                                                  -0.0003
dxy
          -0.0239
                     0.0103
                              -0.0007
                                         -0.0047
dyz
                                                   -0.0084
d3z^2-1
          0.0066
                     0.0085
                               0.0269
                                         0.0181
                                                   0.0136
          -0.0229
                    -0.0096
                              -0.0083
                                         0.0007
                                                   -0.0116
dxz
dx^2-v^2 -0.0058
                     0.0101
                               0.0006
                                         0.0269
                                                   -0.0374
```

Dist=1.7321 Trans. vecs. : 0 1-1								
Connecting vector: 0.000 1.732 0.000								
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2			
dxy	0.0056	0.0108	0.0085	0.0294	0.0010			
dyz	-0.0028	-0.0038	-0.0216	0.0049	-0.0103			
d3z^2-1	-0.0288	0.0200	-0.0001	-0.0132	0.0151			
dxz	0.0106	0.0309	0.0023	-0.0174	0.0250			
dx^2-y^2	-0.0050	-0.0237	-0.0119	-0.0122	0.0047			

Dist=1.7321 Trans. vecs. : 1-1 0							
Connecting vector: 1.500-0.866 0.000							
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2		
dxy	-0.0114	-0.0239	0.0066	-0.0229	-0.0058		
dyz	0.0220	0.0103	0.0085	-0.0096	0.0101		
d3z^2-1	-0.0084	-0.0007	0.0269	-0.0083	0.0006		
dxz	0.0191	-0.0047	0.0181	0.0007	0.0269		
dx^2-y^2	-0.0003	-0.0084	0.0136	-0.0116	-0.0374		

Dist=1.7321 Trans. vecs. : 1 0-1						
Connecti	ng vector:	1.500 0.86	6 0.000			
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2	
dxy	0.0021	0.0030	0.0157	-0.0313	-0.0081	
dyz	-0.0101	8000.0	0.0142	0.0173	0.0183	
d3z^2-1	-0.0299	-0.0160	-0.0085	0.0064	0.0086	
dxz	-0.0016	0.0247	-0.0115	-0.0005	-0.0310	
dx^2-y^2	0.0036	0.0185	-0.0233	0.0055	-0.0048	

XY & XZ change sign

Dist=1.7321 Trans. vecs. : 1 0-1							
Connecti	ng vector:	1.500 0.86	66 0.000				
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2		
dxy	0.0021	0.0101	0.0299	-0.0016	-0.0036		
dyz	-0.0030	8000.0	-0.0160	-0.0247	0.0185		
d3z^2-1	-0.0157	0.0142	-0.0085	0.0115	-0.0233		
dxz	-0.0313	-0.0173	-0.0064	-0.0005	-0.0055		
dx^2-v^2	0.0081	0.0183	0.0086	0.0310	-0.0048		

Co2-Co2

Dist=1.7321 Trans. vecs. : 1-1 0 Connecting vector: 1.500-0.866 0.000								
dxy dyz d3z^2-1 dxz dx^2-y^2	dxy -0.0114 0.0239 -0.0066 -0.0229 0.0058	dyz	d3z^2-1 0.0084 -0.0007 0.0269 0.0083 0.0006	dxz 0.0191 0.0047 -0.0181 0.0007 -0.0269	dx^2-y^2 0.0003 -0.0084 0.0136 0.0116 -0.0374			

		vecs. : 0 1			
Connecti	ng vector:	0.000 1.73	2 0.000		
'	dxy	dyz	d3z^2-1	dxz	dx^2-y^2
dxy	0.0056	0.0028	0.0288	0.0106	0.0050
dyz	-0.0108	-0.0038	0.0200	-0.0309	-0.0237
d3z^2-1	-0.0085	-0.0216	-0.0001	-0.0023	-0.0119
dxz	0.0294	-0.0049	0.0132	-0.0174	0.0122
dx^2-y^2	-0.0010	-0.0103	0.0151	-0.0250	0.0047

```
| IDist=1.7321 Trans. vecs. : 0-1 1
|Connecting vector: 0.000-1.732 0.000
           dxy
                    dyz
                               d3z^2-1
                                          dxz
                                                  dx^2-y^2
dxy
          0.0056
                    -0.0108
                              -0.0085
                                         0.0294
                                                   -0.0010
          0.0028
                    -0.0038
                              -0.0216
                                         -0.0049
                                                   -0.0103
dyz
d3z^2-1
          0.0288
                     0.0200
                              -0.0001
                                         0.0132
                                                   0.0151
           0.0106
                    -0.0309
                              -0.0023
                                         -0.0174
                                                   -0.0250
dx^2-y^2 0.0050
                    -0.0237
                              -0.0119
                                         0.0122
                                                   0.0047
```

```
|Dist=1.7321 Trans. vecs. :-1 1 0
|Connecting vector: -1.500 0.866 0.000
           dxy
                    dyz
                               d3z^2-1
                                         dxz
                                                  dx^2-y^2
                                         -0.0229
          -0.0114
                     0.0239
                               -0.0066
                                                    0.0058
dxy
          -0.0220
                     0.0103
                               0.0085
                                         0.0096
                                                   0.0101
dyz
d3z^2-1
          0.0084
                    -0.0007
                               0.0269
                                         0.0083
                                                    0.0006
dxz
           0.0191
                     0.0047
                              -0.0181
                                         0.0007
                                                   -0.0269
dx^2-y^2
           0.0003
                    -0.0084
                               0.0136
                                          0.0116
                                                   -0.0374
```

```
|Dist=1.7321 Trans. vecs. :-1 0 1
|Connecting vector: -1.500-0.866 0.000
           dxy
                   dyz
                               d3z^2-1
                                         dxz
                                                 dx^2-y^2
          0.0021
                              -0.0157
                                        -0.0313
                                                   0.0081
dxy
                    -0.0030
          0.0101
                    0.0008
                               0.0142
                                        -0.0173
                                                   0.0183
dyz
d3z^2-1
          0.0299
                    -0.0160
                              -0.0085
                                        -0.0064
                                                   0.0086
          -0.0016
                                        -0.0005
                                                   0.0310
dxz
                    -0.0247
                               0.0115
dx^2-v^2 -0.0036
                               -0.0233
                                         -0.0055
                                                   -0.0048
                     0.0185
```

3-6-4.out_rotation

Co2-Co1 & Co1-Co2 hopping matrices (H3) eV unit

Co-Co Bond length: 5.6090 (Å) Numbers: 3 Hopping matrix: H3

Co2-Co1

Co1-Co2

Int.bet. Co1- 3/Co1- 2 Dist=2.0009 Trans. vecs. :-1 1 1 Connecting vector: -2.000 0.000-0.059							
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2		
dxy	0.0276	-0.0208	-0.0233	-0.0056	-0.0066		
dyz	0.0208	-0.0118	-0.0054	0.0024	-0.0211		
d3z^2-1	0.0233	-0.0054	-0.0072	-0.0348	0.0172		
dxz	-0.0056	-0.0024	0.0348	-0.0038	0.0639		
dx^2-y^2	0.0066	-0.0211	0.0172	-0.0639	0.1013		

Dist=2.00	:01- 2/C01- 009 Trans.	vecs.: 1-1				
Connecti	ng vector:	2.000 0.00	00 0.059			
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2	
dxy	0.0276	0.0208	0.0233	-0.0056	0.0066	
dyz	-0.0208	-0.0118	-0.0054	-0.0024	-0.0211	
d3z^2-1	-0.0233	-0.0054	-0.0072	0.0348	0.0172	
dxz	-0.0056	0.0024	-0.0348	-0.0038	-0.0639	
dx^2-y^2	-0.0066	-0.0211	0.0172	0.0639	0.1013	

Int.bet. Co1- 3/Co1- 2 Dist=2.0009 Trans. vecs. : 1-1 1 Connecting vector: 1.000-1.732-0.059							
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2		
dxy	0.0342	0.0222	-0.0116	0.0292	0.0151		
dyz	-0.0222	-0.0062	0.0014	0.0117	0.0200		
d3z^2-1	0.0116	0.0014	0.0121	0.0358	0.0298		
dxz	0.0292	-0.0117	-0.0358	-0.0059	-0.0659		
dx^2-y^2	-0.0151	0.0200	0.0298	0.0659	0.0809		

Int.bet. C	o1- 2/Co1-	- 3			
Dist=2.00	009 Trans.	vecs. :-1 1	-1		
Connecti	ng vector:	-1.000 1.73	2 0.059		
•	dxy	dyz	d3z^2-1	dxz	dx^2-y^2
dxy	0.0342	-0.0222	0.0116	0.0292	-0.0151
dyz	0.0222	-0.0062	0.0014	-0.0117	0.0200
d3z^2-1	-0.0116	0.0014	0.0121	-0.0358	0.0298
dxz	0.0292	0.0117	0.0358	-0.0059	0.0659
dx^2-y^2	0.0151	0.0200	0.0298	-0.0659	0.0809

```
Int.bet. Co1- 3/Co1- 2
|Dist=2.0009 Trans. vecs. : 1 1-1
|Connecting vector: 1.000 1.732-0.059
                             d3z^2-1
                                                dx^2-y^2
           dxy
                   dyz
                                        dxz
         0.0197
                   -0.0014
                             -0.0042
                                       -0.0189
                                                  0.0236
dxy
                   0.0243
                             -0.0044
                                        0.0360
                                                 -0.0084
dyz
         0.0014
d3z^2-1
         0.0042
                             -0.0275
                   -0.0044
                                       -0.0141
                                                  0.0087
dxz
         -0.0189
                   -0.0360
                              0.0141
                                       -0.1278
                                                 -0.0055
                              0.0087
                                        0.0055
dx^2-v^2 -0.0236
                   -0.0084
                                                 -0.0463
```

```
IInt.bet. Co1- 2/Co1- 3
|Dist=2.0009 Trans. vecs. :-1-1 1
|Connecting vector: -1.000-1.732 0.059
                              d3z^2-1
                                        dxz
                                                 dx^2-v^2
           dxv
                     dyz
                    0.0014
                              0.0042
                                        -0.0189
                                                  -0.0236
          0.0197
dxy
          -0.0014
                    0.0243
                              -0.0044
                                        -0.0360
                                                  -0.0084
dvz
          -0.0042
                    -0.0044
                              -0.0275
d3z^2-1
                                         0.0141
                                                   0.0087
          -0.0189
                     0.0360
                              -0.0141
                                         -0.1278
dxz
                                                   0.0055
dx^2-y^2
           0.0236
                     -0.0084
                               0.0087
                                         -0.0055
                                                   -0.0463
```

3-6-4.out rotation

Co2-Co1 & Co1-Co2 hopping matrices (H4) eV unit Co-Co Bond length: 7.4186(Å) Numbers: 6 Hopping matrix: H4

Co2-Co1

Dist=2.6464 Trans. vecs. :-1 0 2							
Connecti	ng vector: -	2.000-1.73	32-0.059				
•	dxy	dyz	d3z^2-1	dxz	dx^2-y^2		
dxy	-0.0019	0.0023	0.0002	0.0011	0.0035		
dyz	-0.0023	0.0013	-0.0016	-0.0001	0.0065		
d3z^2-1	-0.0002	-0.0016	0.0040	0.0011	0.0004		
dxz	0.0011	0.0001	-0.0011	-0.0046	0.0015		
dx^2-y^2	-0.0035	0.0065	0.0004	-0.0015	-0.0055		

```
|Dist=2.6464 Trans. vecs. :-1 2 0
|Connecting vector: -2.000 1.732-0.059
           dxy
                    dyz
                              d3z^2-1
                                        dxz
                                                 dx^2-v^2
          0.0003
                                        0.0029
                    0.0028
                              0.0005
                                                  -0.0046
dxy
         -0.0028
                              -0.0042
                                        -0.0011
                    0.0053
                                                  0.0011
dyz
d3z^2-1
         -0.0005
                    -0.0042
                              0.0017
                                        0.0008
                                                  0.0023
          0.0029
                    0.0011
                             -0.0008
                                        0.0008
                                                  -0.0029
dxz
dx^2-v^2 0.0046
                    0.0011
                              0.0023
                                        0.0029
                                                  -0.0036
```

Dist=2.6464 Trans. vecs. : 0-1 2 Connecting vector: -0.500-2.598-0.059							
dxy	dyz	d3z^2-1	dxz	dx^2-y^2			
-0.0011	-0.0027	0.0014	0.0003	0.0006			
0.0027	0.0021	0.0032	-0.0032	-0.0066			
-0.0014	0.0032	0.0016	-0.0005	0.0009			
0.0003	0.0032	0.0005	-0.0025	0.0003			
-0.0006	-0.0066	0.0009	-0.0003	-0.0051			
	ng vector: dxy -0.0011 0.0027 -0.0014 0.0003	ng vector: -0.500-2.59 dxy dyz -0.0011 -0.0027 0.0027 0.0021 -0.0014 0.0032 0.0003 0.0032	ng vector: -0.500-2.598-0.059 dxy dyz d3z^2-1 -0.0011 -0.0027 0.0014 0.0027 0.0021 0.0032 -0.0014 0.0032 0.0016 0.0003 0.0032 0.0005	ng vector: -0.500-2.598-0.059 dxy dyz d3z^2-1 dxz -0.0011 -0.0027 0.0014 0.0003 0.0027 0.0021 0.0032 -0.0032 -0.0014 0.0032 0.0016 -0.0005 0.0003 0.0032 0.0005 -0.0025	ng vector: -0.500-2.598-0.059 dxy dyz d3z^2-1 dxz dx^2-y^2 -0.0011 -0.0027 0.0014 0.0003 0.0006 0.0027 0.0021 0.0032 -0.0032 -0.0066 -0.0014 0.0032 0.0016 -0.0005 0.0009 0.0003 0.0032 0.0005 -0.0025 0.0003		

Dist=2.6464 Trans. vecs. : 0 2-1							
Connecti	ng vector:	-0.500 2.59	8-0.059				
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2		
dxy	-0.0027	-0.0010	-0.0033	0.0009	-0.0012		
dyz	0.0010	-0.0025	0.0045	-0.0032	0.0004		
d3z^2-1	0.0033	0.0045	0.0009	0.0053	-0.0030		
dxz	0.0009	0.0032	-0.0053	0.0002	-0.0011		
dx^2-y^2	0.0012	0.0004	-0.0030	0.0011	0.0052		

		vecs. : 2-1 2.500-0.86				
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2	
dxy	0.0007	-0.0021	0.0008	-0.0064	-0.0030	
dyz	0.0021	0.0070	0.0014	-0.0003	-0.0003	
d3z^2-1	-0.0008	0.0014	0.0015	-0.0008	0.0026	
dxz	-0.0064	0.0003	0.0008	0.0019	0.0035	
dx^2-y^2	0.0030	-0.0003	0.0026	-0.0035	0.0003	

```
|Dist=2.6464 Trans. vecs. : 2 0-1
|Connecting vector: 2.500 0.866-0.059
                                                  dx^2-y^2
           dxy
                    dyz
                               d3z^2-1
                                         dxz
          -0.0040
                     0.0005
                               -0.0031
                                          0.0001
                                                    0.0001
dxy
          -0.0005
                    -0.0065
                               -0.0019
                                         -0.0041
                                                    0.0004
dyz
d3z^2-1
           0.0031
                     -0.0019
                                0.0048
                                          -0.0042
                                                    -0.0015
                      0.0041
                                0.0042
                                          0.0021
                                                    -0.0004
dxz
           0.0001
dx^2-y^2
           -0.0001
                      0.0004
                                -0.0015
                                          0.0004
                                                     0.0021
```

XY & XZ change sign

```
IDist=2.6464 Trans. vecs.: 1 0-2
IConnecting vector: 2.000 1.732 0.059
                               d3z^2-1
                                         dxz
                                                  dx^2-v^2
           dxy
                    dyz
dxy
          -0.0019
                    -0.0023
                               -0.0002
                                         0.0011
                                                   -0.0035
dyz
           0.0023
                    0.0013
                              -0.0016
                                         0.0001
                                                   0.0065
d3z^2-1
           0.0002
                    -0.0016
                               0.0040
                                        -0.0011
                                                   0.0004
           0.0011
                    -0.0001
                               0.0011
                                        -0.0046
                                                   -0.0015
dxz
dx^2-v^2
           0.0035
                     0.0065
                               0.0004
                                         0.0015
                                                   -0.0055
```

Co1-Co2

```
Dist=2.6464 Trans. vecs.: 1-2 0
|Connecting vector: 2.000-1.732 0.059
                               d3z^2-1
                                                 dx^2-v^2
                   dvz
                                         dxz
           dxv
                   -0.0028
dxy
          0.0003
                             -0.0005
                                        0.0029
                                                  0.0046
dyz
          0.0028
                    0.0053
                             -0.0042
                                        0.0011
                                                  0.0011
d3z^2-1
          0.0005
                   -0.0042
                              0.0017
                                        -0.0008
                                                  0.0023
          0.0029
                   -0.0011
                              0.0008
                                        0.0008
                                                  0.0029
dx^2-y^2 -0.0046
                     0.0011
                               0.0023
                                        -0.0029
                                                   -0.0036
```

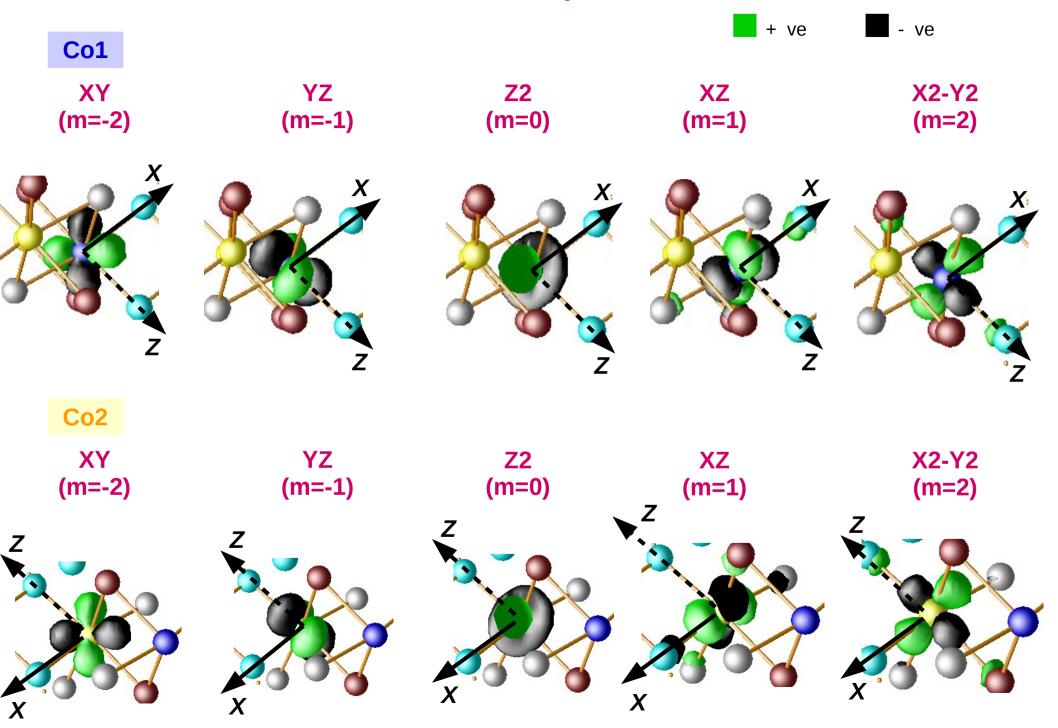
Dist=2.64	164 Trans	. vecs. : 0 2	L-2		
Connecti	ng vector:	0.500 2.59	98 0.059		
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2
dxy	-0.0011	0.0027	-0.0014	0.0003	-0.0006
dyz	-0.0027	0.0021	0.0032	0.0032	-0.0066
d3z^2-1	0.0014	0.0032	0.0016	0.0005	0.0009
dxz	0.0003	-0.0032	-0.0005	-0.0025	-0.0003
dx^2-y^2	0.0006	-0.0066	0.0009	0.0003	-0.0051

```
|Dist=2.6464 Trans. vecs.: 0-2 1
Connecting vector: 0.500-2.598 0.059
           dxy
                    dyz
                               d3z^2-1
                                          dxz
                                                  dx^2-y^2
                               0.0033
                                          0.0009
                                                    0.0012
dxy
          -0.0027
                     0.0010
                    -0.0025
dyz
          -0.0010
                               0.0045
                                          0.0032
                                                    0.0004
d3z^2-1
          -0.0033
                     0.0045
                               0.0009
                                         -0.0053
                                                   -0.0030
           0.0009
                     -0.0032
                                0.0053
                                                    0.0011
                                          0.0002
                     0.0004
                               -0.0030
                                          -0.0011
                                                    0.0052
dx^2-y^2
           -0.0012
```

```
IDist=2.6464 Trans, vecs. :-2 1 0
|Connecting vector: -2.500 0.866 0.059
                              d3z^2-1
                                         dxz
                                                 dx^2-v^2
           dxy
                    dyz
          0.0007
                    0.0021
                              -0.0008
                                                   0.0030
dxy
                                        -0.0064
dyz
          -0.0021
                    0.0070
                              0.0014
                                        0.0003
                                                  -0.0003
d3z^2-1
          0.0008
                    0.0014
                              0.0015
                                        0.0008
                                                   0.0026
dxz
          -0.0064
                    -0.0003
                              -0.0008
                                         0.0019
                                                   -0.0035
dx^2-y^2 -0.0030
                    -0.0003
                               0.0026
                                         0.0035
                                                   0.0003
```

```
|Dist=2.6464 Trans. vecs. :-2 0 1
|Connecting vector: -2.500-0.866 0.059
                    dyz
                               d3z^2-1
                                          dxz
                                                   dx^2-y^2
           dxy
          -0.0040
                    -0.0005
                                0.0031
                                          0.0001
                                                    -0.0001
dxy
                     -0.0065
dyz
           0.0005
                               -0.0019
                                          0.0041
                                                    0.0004
                                0.0048
                                          0.0042
                                                    -0.0015
d3z^2-1
          -0.0031
                     -0.0019
dxz
            0.0001
                     -0.0041
                                -0.0042
                                           0.0021
                                                     0.0004
dx^2-y^2
            0.0001
                      0.0004
                                -0.0015
                                          -0.0004
                                                     0.0021
```

Wannier plots



XY & XZ change sign