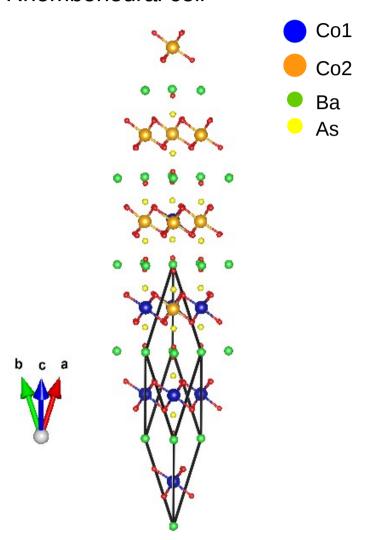
Coordinates, onsite energies, hopping matrices & wannier plots BaCo₂(AsO₄)₂

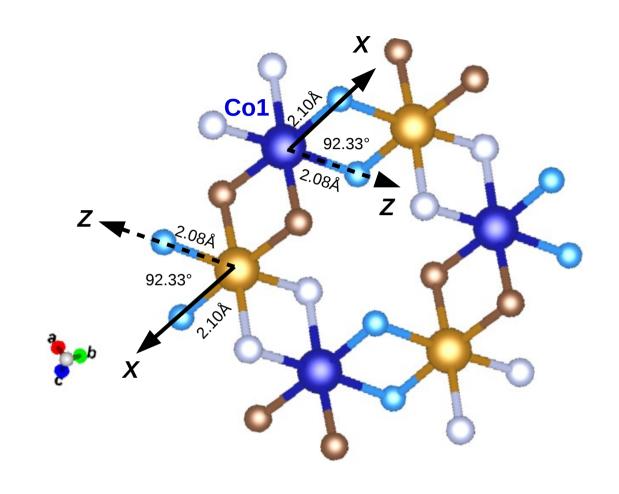
31.1.2021

Coordinate_BaCo₂(AsO₄)₂

Space group: *R-3* (148)





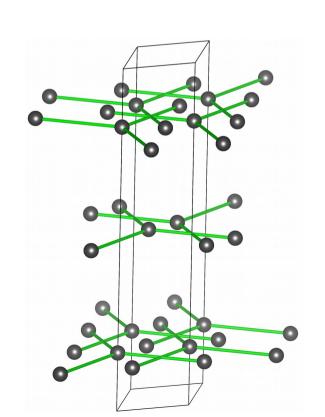


BaCo₂(AsO₄)₂ Co-Co neighbors

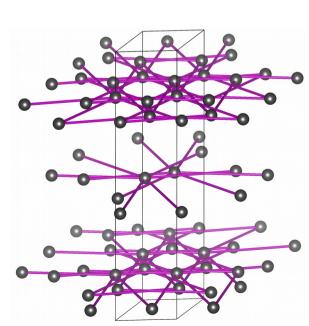
Nearest neighbor & next nearest neighbor

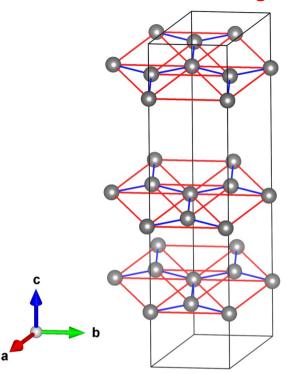
Co-Co Bond-length (Å)	Numbers
2.895	3
5.007	6
5.784	3
7.650	6

5.784Å



7.650Å





Onsite energies eV

Co₁

	dxy	dyz	d3z^2-1	dxz	dx^2-y^2
dxy	-2.8610	-0.0005	-0.0495	0.0124	0.0490
dyz	-0.0005	-2.9578	0.0123	0.0140	0.0202
d3z^2-1	-0.0495	0.0123	-2.6055	-0.0043	0.5312
dxz	0.0124	0.0140	-0.0043	-1.6838	0.0020
dx^2-y^2	0.0490	0.0202	0.5312	0.0020	-1.9904

Co₂

	dxy	dyz	d3z^2-1	dxz c	lx^2-y^2
dxy	-2.8610	0.0005	0.0495	0.0124	-0.0490
dyz	0.0005	-2.9578	0.0123	-0.0140	0.0202
d3z^2-1	0.0495	0.0123	-2.6055	0.0043	0.5312
dxz	0.0124	-0.0140	0.0043	-1.6838	-0.0020
dx^2-y^2	-0.0490	0.0202	0.5312	-0.0020	-1.9904

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

Co-Co Bond length: 2.895 (Å) Numbers: 3 Hopping matrix: H1

Co2-Co1

Int.bet. Co1- 3/Co1- 2 Dist=1.0016 Trans. vecs. : 0 0 1 Connecting vector: -0.500-0.866-0.056						
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2	
dxy	0.0883	0.1892	-0.0012	-0.0676	0.0240	
dyz	-0.1892	-0.1539	0.0095	0.0133	-0.0808	
d3z^2-1	0.0012	0.0095	0.0176	-0.0115	-0.0560	
dxz	-0.0676	-0.0133	0.0115	0.0250	-0.0087	
dx^2-y^2	-0.0240	-0.0808	-0.0560	0.0087	0.0292	

Int.bet. Co1- 3/Co1- 2 Dist=1.0016 Trans. vecs. : 0 1 0 Connecting vector: -0.500 0.866-0.056						
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2	
dxy	0.0849	-0.1913	-0.0034	0.0711	0.0005	
dyz	0.1913	-0.1581	-0.0147	0.0391	0.0531	
d3z^2-1	0.0034	-0.0147	0.0038	0.0034	-0.0649	
dxz	0.0711	-0.0391	-0.0034	0.0226	0.0043	
dx^2-y^2	-0.0005	0.0531	-0.0649	-0.0043	0.0416	

Int.bet. Co1- 3/Co1- 2 Dist=1.0016 Trans. vecs. : 1 0 0 Connecting vector: 1.000 0.000-0.056							
Connectir	ig vector:	1.000 0.00	10-0.056				
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2		
dxy	-0.0442	0.0009	-0.0476	0.0076	0.0052		
dyz	-0.0009	0.0961	-0.0033	-0.0558	0.0123		
d3z^2-1	0.0476	-0.0033	-0.1699	0.0221	0.1650		
dxz	0.0076	0.0558	-0.0221	0.0240	0.0129		
dx^2-y^2	-0.0052	0.0123	0.1650	-0.0129	-0.1668		

Co1-Co2

Int.bet. Co1- 2/Co1- 3 Dist=1.0016 Trans. vecs. : 0 0-1 Connecting vector: 0.500 0.866 0.056						
dxy dyz d3z^2-1 dxz dx^2-y^2	dxy 0.0883 0.1892 -0.0012 -0.0676 0.0240	dyz -0.1892 -0.1539 0.0095 0.0133 -0.0808	d3z^2-1 0.0012 0.0095 0.0176 -0.0115 -0.0560	dxz -0.0676 -0.0133 0.0115 0.0250 -0.0087	dx^2-y^2 -0.0240 -0.0808 -0.0560 0.0087 0.0292	

Int.bet. Co1- 2/Co1- 3 Dist=1.0016 Trans. vecs. : 0-1 0 Connecting vector: 0.500-0.866 0.056							
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2		
dxy	0.0849	0.1913	0.0034	0.0711	-0.0005		
dyz	-0.1913	-0.1581	-0.0147	-0.0391	0.0531		
d3z^2-1	-0.0034	-0.0147	0.0038	-0.0034	-0.0649		
dxz	0.0711	0.0391	0.0034	0.0226	-0.0043		
dx^2-y^2	0.0005	0.0531	-0.0649	0.0043	0.0416		

Int.bet. Co1- 2/Co1- 3 Dist=1.0016 Trans. vecs. :-1 0 0 Connecting vector: -1.000 0.000 0.056							
Connectin	ig vector: -	$\cdot 1.000 \ 0.00$	0.056				
	dxy	dyz	d3z^2-1	dxz c	lx^2-y^2		
dxy	-0.0442	-0.0009	0.0476	0.0076	-0.0052		
dyz	0.0009	0.0961	-0.0033	0.0558	0.0123		
d3z^2-1	-0.0476	-0.0033	-0.1699	-0.0221	0.1650		
dxz	0.0076	-0.0558	0.0221	0.0240	-0.0129		
dx^2-y^2	0.0052	0.0123	0.1650	0.0129	-0.1668		

3-6-4.out rotation

Co1-Co1 & Co2-Co2 hopping matrices (H2) eV unit Numbers: 6 Co-Co Bond length: 5.007(Å) **Hopping matrix: H2**

Co1-Co1

```
Co2-Co2
                                                                                                                Dist=1.7321 Trans. vecs.: 10-1
Dist=1.7321 Trans. vecs. :-1 0 1
                                                                                                                Connecting vector: 1.500 0.866 0.000
Connecting vector: -1.500-0.866 0.000
                                                                                                                                   dyz
                                                                                                                                              d3z^2-1
                                                                                                                                                         dxz
                                                                                                                                                                 dx^2-v^2
                                                                                                                           dxy
           dxy
                   dvz
                               d3z^2-1
                                         dxz
                                                  dx^2-y^2
                                                                                                                                              -0.0082
                                                                                                                                                        -0.0364
                                                                                                                                                                  -0.0053
                                                                                                                dxy
                                                                                                                           0.0034
                                                                                                                                    -0.0012
           0.0034
                    0.0012
                               0.0082
                                        -0.0364
                                                   0.0053
dxv
                                                                                                                dyz
                                                                                                                           0.0009
                                                                                                                                    0.0003
                                                                                                                                              0.0111
                                                                                                                                                         0.0081
                                                                                                                                                                   0.0097
          -0.0009
                    0.0003
                               0.0111
                                        -0.0081
                                                   0.0097
                                                                                                                d3z^2-1
dyz
                                                                                                                          -0.0259
                                                                                                                                    -0.0195
                                                                                                                                               0.0058
                                                                                                                                                         0.0202
                                                                                                                                                                   0.0095
d3z^2-1
          0.0259
                    -0.0195
                               0.0058
                                        -0.0202
                                                   0.0095
                                                                                                                          -0.0165
                                                                                                                                     0.0337
                                                                                                                                              -0.0090
                                                                                                                                                         0.0014
                                                                                                                                                                  -0.0084
                                                                                                                dxz
dxz
          -0.0165
                    -0.0337
                               0.0090
                                         0.0014
                                                   0.0084
                                                                                                                dx^2-v^2
                                                                                                                           0.0010
                                                                                                                                     0.0355
                                                                                                                                              -0.0133
                                                                                                                                                         0.0134
                                                                                                                                                                   0.0094
dx^2-y^2
         -0.0010
                     0.0355
                               -0.0133
                                         -0.0134
                                                   0.0094
                                                                                                               Dist=1.7321 Trans. vecs.: 1-10
Dist=1.7321 Trans. vecs. :-1 1 0
                                                                                                               Connecting vector: 1.500-0.866 0.000
Connecting vector: -1.500 0.866 0.000
                                                                                                                           dxy
                                                                                                                                   dyz
                                                                                                                                              d3z^2-1
                                                                                                                                                         dxz
                                                                                                                                                                 dx^2-v^2
                                                  dx^2-y^2
           dxy
                   dyz
                              d3z^2-1
                                        dxz
                                                                                                                                              -0.0026
                                                                                                                                                                  -0.0103
                                                                                                               dxy
                                                                                                                          0.0064
                                                                                                                                   -0.0100
                                                                                                                                                         0.0367
           0.0064
                    0.0100
                               0.0026
                                         0.0367
                                                   0.0103
dxy
                                                                                                                          0.0046
                                                                                                                                    0.0032
                                                                                                                                              -0.0069
                                                                                                                                                         0.0170
                                                                                                                                                                  -0.0149
                                                                                                               dyz
dyz
           -0.0046
                     0.0032
                               -0.0069
                                         -0.0170
                                                   -0.0149
                                                                                                               d3z^2-1
                                                                                                                         -0.0300
                                                                                                                                    0.0171
                                                                                                                                              -0.0043
                                                                                                                                                        -0.0180
                                                                                                                                                                   0.0079
d3z^2-1
           0.0300
                     0.0171
                               -0.0043
                                         0.0180
                                                   0.0079
                                                                                                                          0.0114
                                                                                                                                    0.0300
                                                                                                                                              0.0139
                                                                                                                                                                   0.0110
                                                                                                               dxz
                                                                                                                                                        0.0107
dxz
           0.0114
                     -0.0300
                               -0.0139
                                          0.0107
                                                   -0.0110
                                                                                                               dx^2-v^2
                                                                                                                          0.0055
                                                                                                                                    -0.0298
                                                                                                                                              -0.0177
                                                                                                                                                        -0.0078
                                                                                                                                                                   0.0043
dx^2-v^2
           -0.0055
                      -0.0298
                                -0.0177
                                          0.0078
                                                    0.0043
                                                                                                               Dist=1.7321 Trans. vecs.: 0 1-1
Dist=1.7321 Trans. vecs.: 0-1 1
                                                                                                               Connecting vector: 0.000 1.732 0.000
Connecting vector: 0.000-1.732 0.000
                                                                                                                                              d3z^2-1
                                                                                                                                                                 dx^2-v^2
                                                                                                                          dxy
                                                                                                                                   dyz
                                                                                                                                                        dxz
           dxy
                   dyz
                               d3z^2-1
                                          dxz
                                                   dx^2-y^2
                                                                                                                                             -0.0051
                                                                                                                                                        -0.0071
                                                                                                                                                                  0.0002
                                                                                                               dxy
                                                                                                                         -0.0153
                                                                                                                                   -0.0177
                               0.0051
                                        -0.0071
                                                  -0.0002
dxy
          -0.0153
                    0.0177
                                                                                                               dyz
                                                                                                                         0.0228
                                                                                                                                   0.0253
                                                                                                                                              0.0042
                                                                                                                                                       -0.0073
                                                                                                                                                                  0.0173
          -0.0228
                    0.0253
                               0.0042
                                         0.0073
                                                   0.0173
dyz
                                                                                                               d3z^2-1
                                                                                                                         0.0067
                                                                                                                                   -0.0063
                                                                                                                                              0.0368
                                                                                                                                                       -0.0135
                                                                                                                                                                  0.0255
d3z^2-1
          -0.0067
                    -0.0063
                               0.0368
                                         0.0135
                                                   0.0255
                                                                                                                                   -0.0071
                                                                                                                                              0.0071
                                                                                                                                                        0.0011
                                                                                                               dxz
                                                                                                                          0.0111
                                                                                                                                                                  0.0085
          0.0111
                    0.0071
                              -0.0071
                                         0.0011
                                                  -0.0085
dxz
                                                                                                               dx^2-y^2 -0.0030
                                                                                                                                   -0.0202
                                                                                                                                              0.0177
                                                                                                                                                       -0.0185
                                                                                                                                                                 -0.0277
dx^2-v^2
          0.0030
                    -0.0202
                              0.0177
                                         0.0185
                                                  -0.0277
                                                                                                               Dist=1.7321 Trans. vecs.: 0-11
                                                                                                               Connecting vector: 0.000-1.732 0.000
                                                                                                                          dxy
                                                                                                                                  dyz
                                                                                                                                              d3z^2-1
                                                                                                                                                        dxz
                                                                                                                                                                 dx^2-y^2
                                                                                                                         -0.0153
                                                                                                                                              0.0067
                                                                                                                                                        0.0111
                                                                                                                                                                 -0.0030
                                                                                                               dxy
                                                                                                                                   0.0228
```

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			
-0.0153	-0.0228	-0.0067	0.0111	0.0030			
0.0177	0.0253	-0.0063	0.0071	-0.0202			
0.0051	0.0042	0.0368	-0.0071	0.0177			
-0.0071	0.0073	0.0135	0.0011	0.0185			
-0.0002	0.0173	0.0255	-0.0085	-0.0277			
	dxy -0.0153 0.0177 0.0051 -0.0071	g vector: 0.000 1.73; dxy dyz -0.0153 -0.0228 0.0177 0.0253 0.0051 0.0042 -0.0071 0.0073	g vector: 0.000 1.732 0.000 dxy dyz d3z^2-1 -0.0153 -0.0228 -0.0067 0.0177 0.0253 -0.0063 0.0051 0.0042 0.0368 -0.0071 0.0073 0.0135	g vector: 0.000 1.732 0.000 dxy dyz d3z^2-1 dxz -0.0153 -0.0228 -0.0067 0.0111 0.0177 0.0253 -0.0063 0.0071 0.0051 0.0042 0.0368 -0.0071 -0.0071 0.0073 0.0135 0.0011	g vector: 0.000 1.732 0.000 dxy dyz d3z^2-1 dxz dx^2-y^2 -0.0153 -0.0228 -0.0067 0.0111 0.0030 0.0177 0.0253 -0.0063 0.0071 -0.0202 0.0051 0.0042 0.0368 -0.0071 0.0177 -0.0071 0.0073 0.0135 0.0011 0.0185		

Dist=1.7321 Trans. vecs. : 1-1 0 Connecting vector: 1.500-0.866 0.000							

DISI-1.7321 Halls. Vecs 1 U-1								
Connecting vector: 1.500 0.866 0.000								
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2			
dxy	0.0034	-0.0009	0.0259	-0.0165	-0.0010			
dyz	0.0012	0.0003	-0.0195	-0.0337	0.0355			
d3z^2-1	0.0082	0.0111	0.0058	0.0090	-0.0133			
dxz	-0.0364	-0.0081	-0.0202	0.0014	-0.0134			
dx^2-y^2	0.0053	0.0097	0.0095	0.0084	0.0094			

Diot-1 7221 Tropo voco : 1 0 1

XY & XZ change sign

0.0253 -0.0063-0.0071 dyz -0.0177 -0.0202d3z^2-1 -0.0051 0.0042 0.0368 0.0071 0.0177 -0.0071-0.0073 -0.0135 0.0011 -0.0185 dxz dx^2-y^2 0.0002 0.0173 0.0255 0.0085 -0.0277Dist=1.7321 Trans. vecs. :-1 1 0 Connecting vector: -1.500 0.866 0.000 dxv d3z^2-1 dxz dx^2-y^2 dyz 0.0064 0.0046 -0.0300 0.0114 0.0055 dxy -0.0100 0.0032 0.0171 0.0300 -0.0298dvz d3z^2-1 -0.0026 -0.0069 -0.00430.0139 -0.01770.0367 0.0170 -0.0180 0.0107 -0.0078 dx^2-v^2 -0.0103 -0.0149 0.0079 0.0110 0.0043 Dist=1.7321 Trans. vecs. :-1 0 1

d3z^2-1

-0.0259

-0.0195

0.0058

0.0202

0.0095

dxz

-0.0165

0.0337

-0.0090

0.0014

-0.0084

dx^2-y^2

0.0010

0.0355

-0.0133

0.0134

0.0094

Connecting vector: -1.500-0.866 0.000

dyz

0.0009

0.0003

0.0111

0.0081

0.0097

dxy

dxy

dyz d3z^2-1

dxz

0.0034

-0.0012

-0.0082

-0.0364

 $dx^2-y^2 -0.0053$

Int.bet. Co1- 2/Co1- 3

3-6-4.out_rotation

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

Co-Co Bond length: 5.784(Å)

Numbers: 3 Hopping matrix: H3

Co2-Co1

Co1-Co2

Int.bet. Co1- 3/Co1- 2									
Dist=2.00	Dist=2.0008 Trans. vecs. :-1 1 1								
Connecting vector: -2.000 0.000-0.056									
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2				
dxy	0.0027	-0.0007	0.0015	0.0134	-0.0086				
dyz	0.0007	0.0061	0.0000	-0.0137	0.0077				
d3z^2-1	-0.0015	0.0000	-0.0258	-0.0078	0.0149				
dxz	0.0134	0.0137	0.0078	-0.1327	-0.0042				
dx^2-y^2	0.0086	0.0077	0.0149	0.0042	-0.0646				

	Dist=2.0008 Trans. vecs. : 1-1-1								
	Connecting vector: 2.000 0.000 0.056								
		dxy	dyz	d3z^2-1	dxz	dx^2-y^2			
	dxy	0.0027	0.0007	-0.0015	0.0134	0.0086			
	dyz	-0.0007	0.0061	0.0000	0.0137	0.0077			
	d3z^2-1	0.0015	0.0000	-0.0258	0.0078	0.0149			
	dxz	0.0134	-0.0137	-0.0078	-0.1327	0.0042			
	dx^2-y^2	-0.0086	0.0077	0.0149	-0.0042	-0.0646			
ſ									
	Int.bet. Co1- 2/Co1- 3								

Dist=2.0008 Trans. vecs. : 1-1 1 Connecting vector: 1.000-1.732-0.056							
Connectir	ng vector:	1.000-1.73	32-0.056				
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2		
dxy	0.0242	-0.0243	0.0151	0.0084	0.0129		
dyz	0.0243	-0.0226	0.0094	0.0107	0.0141		
d3z^2-1	-0.0151	0.0094	0.0051	-0.0363	0.0260		
dxz	0.0084	-0.0107	0.0363	-0.0019	0.0661		
dx^2-y^2	-0.0129	0.0141	0.0260	-0.0661	0.0856		

Int.bet. Co1- 2/Co1- 3 Dist=2.0008 Trans. vecs. :-1 1-1 Connecting vector: -1.000 1.732 0.056								
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2			
dxy	0.0242	0.0243	-0.0151	0.0084	-0.0129			
dyz	-0.0243	-0.0226	0.0094	-0.0107	0.0141			
d3z^2-1	0.0151	0.0094	0.0051	0.0363	0.0260			
dxz	0.0084	0.0107	-0.0363	-0.0019	-0.0661			
dx^2-y^2	0.0129	0.0141	0.0260	0.0661	0.0856			

Int.bet. Co1- 3/Co1- 2							
Dist=2.00	08 Trans.	vecs.: 1 1-	-1				
Connectir	ng vector:	1.000 1.73	2-0.056				
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2		
dxy	0.0283	0.0255	-0.0005	-0.0298	-0.0060		
dyz	-0.0255	-0.0177	-0.0026	0.0075	-0.0102		
d3z^2-1	0.0005	-0.0026	0.0251	0.0377	0.0394		
dxz	-0.0298	-0.0075	-0.0377	-0.0013	-0.0658		
dx^2-y^2	0.0060	-0.0102	0.0394	0.0658	0.0653		

Int.bet. Co1- 2/Co1- 3 Dist=2.0008 Trans. vecs. :-1-1 1 Connecting vector: -1.000-1.732 0.056								
	dxy	dyz		dxz	dx^2-y^2			
dxy	0.0283	-0.0255	0.0005	-0.0298	0.0060			
dyz	0.0255	-0.0177	-0.0026	-0.0075	-0.0102			
d3z^2-1	-0.0005	-0.0026	0.0251	-0.0377	0.0394			
dxz	-0.0298	0.0075	0.0377	-0.0013	0.0658			
dx^2-y^2	-0.0060	-0.0102	0.0394	-0.0658	0.0653			

3-6-4.out_rotation

Co-Co Bond length: 7.650(Å) Numbers: 6 Honning matrix: L4

	-			- 4	 2	 	. •	$\mathbf{\circ}$	$\mathbf{\circ}$	•	`'	_
•	^	2		01						•	•	- (
	L J	_	-	·								_

Dist=2.6464 Trans. vecs. :-1 0 2 Connecting vector: -2.000-1.732-0.056							
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2		
dxy	-0.0023	0.0003	0.0049	0.0006	-0.0001		
dyz	-0.0003	-0.0041	-0.0050	0.0041	0.0009		
d3z^2-1	-0.0049	-0.0050	-0.0006	0.0102	-0.0030		
dxz	0.0006	-0.0041	-0.0102	-0.0004	-0.0041		
dx^2-y^2	0.0001	0.0009	-0.0030	0.0041	0.0090		

```
Dist=2.6464 Trans. vecs.: 10-2
Connecting vector: 2.000 1.732 0.056
           dxy
                   dyz
                             d3z^2-1
                                       dxz
                                                 dx^2-v^2
          -0.0023
                  -0.0003
                             -0.0049
                                        0.0006
                                                  0.0001
dxy
dyz
          0.0003
                   -0.0041
                             -0.0050
                                       -0.0041
                                                  0.0009
d3z^2-1
          0.0049
                   -0.0050
                              -0.0006
                                       -0.0102
                                                 -0.0030
          0.0006
                    0.0041
                              0.0102
                                       -0.0004
                                                  0.0041
dxz
dx^2-v^2 -0.0001
                    0.0009
                              -0.0030
                                       -0.0041
                                                  0.0090
```

Dist=2.6464 Trans. vecs. :-1 2 0 Connecting vector: -2.000 1.732-0.056 dxy d3z^2-1 dx^2-y^2 dyz dxz -0.0014 -0.0034 -0.0002 0.0048 -0.0010 dxy 0.0002 -0.0065 0.0032 0.0062 -0.0027 dyz d3z^2-1 -0.0048 0.0032 0.0047 -0.0109-0.0013 -0.0010 -0.0062 0.0109 0.0008 dxz 0.0011 dx^2-v^2 0.0014 -0.0027 -0.0013 -0.0008 0.0035

```
Dist=2.6464 Trans. vecs.: 1-2 0
Connecting vector: 2.000-1.732 0.056
                                                 dx^2-v^2
                     dyz
                              d3z^2-1
           dxy
                                        dxz
          -0.0034
                     0.0002
                              -0.0048
                                        -0.0010
                                                  0.0014
dxy
          -0.0002
                    -0.0065
                               0.0032
                                        -0.0062
                                                  -0.0027
dyz
d3z^2-1
           0.0048
                     0.0032
                               0.0047
                                        0.0109
                                                  -0.0013
dxz
          -0.0010
                     0.0062
                              -0.0109
                                         0.0011
                                                  -0.0008
dx^2-y^2 -0.0014
                    -0.0027
                              -0.0013
                                         0.0008
                                                   0.0035
```

Dist=2.6464 Trans. vecs. : 0-1 2								
Connecting vector: -0.500-2.598-0.056								
	dxy dyz d3z^2-1 dxz dx^2-y^2							
dxy	0.0038	0.0038	0.0013	-0.0045	0.0083			
dyz	-0.0038	0.0083	0.0050	-0.0015	0.0007			
d3z^2-1	-0.0013	0.0050	0.0047	0.0012	0.0054			
dxz	-0.0045	0.0015	-0.0012	0.0037	-0.0050			
dx^2-y^2	-0.0083	0.0007	0.0054	0.0050	-0.0016			

	Dist=2.6464 Trans. vecs. : 0 1-2								
Connectin	Connecting vector: 0.500 2.598 0.056								
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2				
dxy	0.0038	-0.0038	-0.0013	-0.0045	-0.0083				
dyz	0.0038	0.0083	0.0050	0.0015	0.0007				
d3z^2-1	0.0013	0.0050	0.0047	-0.0012	0.0054				
dxz	-0.0045	-0.0015	0.0012	0.0037	0.0050				
dx^2-y^2	0.0083	0.0007	0.0054	-0.0050	-0.0016				

```
Dist=2.6464 Trans. vecs.: 0 2-1
Connecting vector: -0.500 2.598-0.056
                             d3z^2-1
                                                dx^2-y^2
          dxy
                   dyz
                                       dxz
                   -0.0026
                             -0.0005
                                       0.0084
                                                 0.0036
dxy
          0.0050
          0.0026
                   0.0080
                             -0.0027
                                       -0.0033
                                                 -0.0003
dyz
d3z^2-1
         0.0005
                   -0.0027
                             0.0045
                                      -0.0020
                                                 0.0056
                   0.0033
                             0.0020
                                       0.0043
                                                 0.0058
          0.0084
dxz
dx^2-y^2 -0.0036
                   -0.0003
                              0.0056
                                       -0.0058
                                                0.0038
```

Dist=2.6464 Trans. vecs. : 0-2 1								
Connecting vector: 0.500-2.598 0.056								
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2			
dxy	0.0050	0.0026	0.0005	0.0084	-0.0036			
dyz	-0.0026	0.0080	-0.0027	0.0033	-0.0003			
d3z^2-1	-0.0005	-0.0027	0.0045	0.0020	0.0056			
dxz	0.0084	-0.0033	-0.0020	0.0043	-0.0058			
dx^2-y^2	0.0036	-0.0003	0.0056	0.0058	0.0038			

Dist=2.6464 Trans. vecs. : 2-1 0 Connecting vector: 2.500-0.866-0.056								
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2			
dxy	-0.0018	0.0021	-0.0002	-0.0027	-0.0052			
dyz	-0.0021	0.0015	0.0019	0.0002	-0.0104			
d3z^2-1	0.0002	0.0019	0.0006	-0.0002	-0.0003			
dxz	-0.0027	-0.0002	0.0002	-0.0106	0.0032			
dx^2-y^2	0.0052	-0.0104	-0.0003	-0.0032	-0.0075			

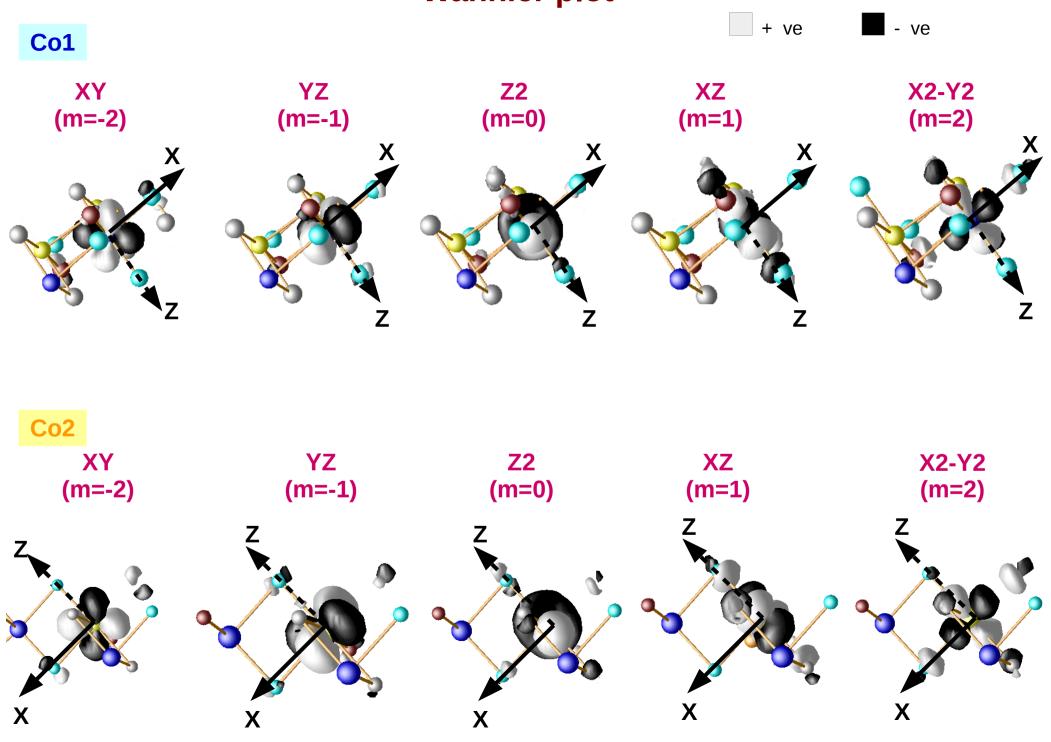
```
Dist=2.6464 Trans. vecs. :-2 1 0
Connecting vector: -2.500 0.866 0.056
                                                  dx^2-y^2
           dxy
                    dyz
                               d3z^2-1
                                         dxz
dxy
          -0.0018
                    -0.0021
                               0.0002
                                        -0.0027
                                                   0.0052
          0.0021
                    0.0015
                               0.0019
                                        -0.0002
                                                  -0.0104
dyz
          -0.0002
                     0.0019
                                                  -0.0003
d3z^2-1
                               0.0006
                                         0.0002
          -0.0027
                     0.0002
                              -0.0002
                                        -0.0106
                                                  -0.0032
dx^2-y^2 -0.0052
                    -0.0104
                              -0.0003
                                         0.0032
                                                  -0.0075
```

Dist=2.6464 Trans. vecs. : 2 0-1						
Connecting vector: 2.500 0.866-0.056						
	dxy	dyz	d3z^2-1	dxz	dx^2-y^2	
dxy	-0.0013	-0.0034	-0.0006	-0.0005	-0.0029	
dyz	0.0034	0.0028	-0.0027	0.0060	0.0110	
d3z^2-1	0.0006	-0.0027	0.0004	0.0021	-0.0001	
dxz	-0.0005	-0.0060	-0.0021	-0.0070	-0.0002	
dx^2-y^2	0.0029	0.0110	-0.0001	0.0002	-0.0076	
						_

```
Dist=2.6464 Trans. vecs. :-2 0 1
Connecting vector: -2.500-0.866 0.056
          dxy
                   dyz
                              d3z^2-1
                                        dxz
                                                 dx^2-y^2
         -0.0013
                    0.0034
                              0.0006
                                       -0.0005
                                                  0.0029
dxy
         -0.0034
                    0.0028
                              -0.0027
                                       -0.0060
                                                  0.0110
dyz
d3z^2-1 -0.0006
                   -0.0027
                              0.0004
                                       -0.0021
                                                  -0.0001
         -0.0005
                    0.0060
                              0.0021
                                       -0.0070
                                                  0.0002
dxz
dx^2-y^2 -0.0029
                    0.0110
                              -0.0001
                                       -0.0002
                                                  -0.0076
```

XY & XZ change sign

Wannier plot



XY & XZ change sign