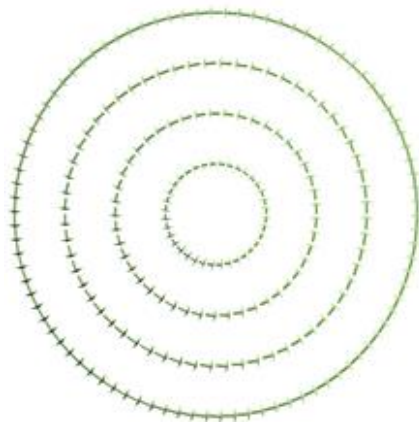
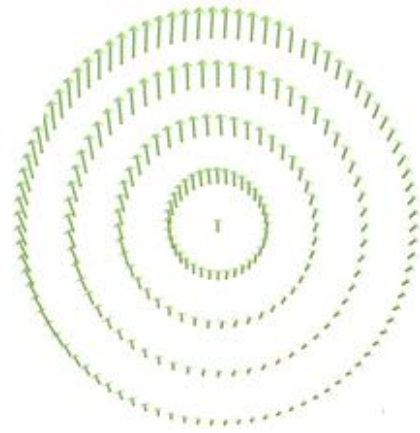


Black bands – band structure from VASP code; Red bands – band structure from output file (wannier90_band.dat) from WANNIER90 code; Blue bands – band structure from the Hamiltonian extract from wannier90_hr.dat by my code



Spin texture from VASP code



Spin texture from Hamiltonian extracted from WANNIER90 code by my code

Parameter settings in DFT calculation based on VASP code:

Syetem = Graphene_3LCo_Graphene

ISTART = 1

LWAVE = .TRUE.

LCHARGE = .TRUE.

ICHARG = 11

IVDW = 12

ISPIN = 1

LMAXMIX = 4

```
LNONCOLLINEAR = .TRUE.
LSORBIT = .TRUE.
LORBMOM = .TRUE.
GGA_COMPAT = .FALSE.
ENCUT = 620
ISM EAR = 1
SIGMA = 0.01
NBANDS = 96
PREC = Accurate
MAGMOM = 0 0 0 0 0 0 0 3 0 0 3 0 0 3
I_CONSTRAINED_M = 1
RWIGS = 1.0 2.0
LAMBDA = 10
M_CONSTR = 0 0 0 0 0 0 0 0 1 0 0 1 0 0 1
LREAL = .FALSE.
LORBIT = 11
NELMIN = 5
NELM = 700
NELMDL = -10
EDIFF = 1e-7
```

Parameter settings in 'wannier90.win' file:

```
num_wann = 46
num_bands = 96
num_iter = 1000
dis_num_iter = 2000
guiding_centres = .true.
begin projections
C : pz
Co : px; py; dz2; dxz; dyz; dxy; dx2-y2;z=0,0,1:(u,d)[0,0,1]
end projections
spinors = .true.
```

```

write_hr = true
dis_froz_min = -2.6681
dis_froz_max = 1.3319
dis_win_max = 10.5248
dis_win_min = -16.5
exclude_bands : 1-6
slwf_constrain = true
slwf_lambda = 3
begin unit_cell_cart
  2.5070000  0.0000000  0.0000000
 -1.2535000  2.1711257  0.0000000
  0.0000000  0.0000000  32.0190010
end unit_cell_cart
begin atoms_cart
C   1.2535000  0.7237086  8.1691010
C   0.0000000  0.0000000  8.1691010
Co  1.2535000  0.7237086  2.2983135
Co  -0.0000000  1.4474171  4.2147650
Co  1.2535000  0.7237086  6.1691010
end atoms_cart
bands_plot = .true.
bands_num_points = 200
begin kpoint_path
K6 -0.3333333333 0.6666666667 0.0000000000 K1 0.3333333333 0.3333333333 0.0000000000
K1 0.3333333333 0.3333333333 0.0000000000 K2 0.6666666667 -0.3333333333 0.0000000000
end kpoint_path
bands_plot_format = gnuplot xmgrace
mp_grid = 41 41 1
begin kpoints
  0.000000000000  0.000000000000  0.000000000000
  0.024390243902  0.000000000000  0.000000000000
  0.048780487805  0.000000000000  0.000000000000

```

0.073170731707	0.000000000000	0.000000000000
.....		
-0.365853658537	0.682926829268	0.000000000000
0.658536585366	-0.292682926829	0.000000000000
-0.365853658537	0.658536585366	0.000000000000
0.682926829268	-0.341463414634	0.000000000000
-0.341463414634	0.682926829268	0.000000000000

end kpoints

Output in 'wannier90.wout' file:

Final State

WF centre and spread	1	(1.253092, 0.722674, 8.177711)	1.13296686
WF centre and spread	2	(-0.000493, -0.002853, 8.240137)	1.06617677
WF centre and spread	3	(1.191006, 1.856331, 1.800273)	8.11287824
WF centre and spread	4	(1.332159, 1.860353, 1.125323)	8.08293679
WF centre and spread	5	(1.253412, 0.720057, 2.254204)	0.52810684
WF centre and spread	6	(1.250568, 0.726713, 2.306737)	0.54321583
WF centre and spread	7	(1.255375, 0.724237, 2.318336)	0.54528533
WF centre and spread	8	(1.250972, 0.749589, 2.297542)	0.56777492
WF centre and spread	9	(1.254268, 0.684527, 2.297424)	0.64605760
WF centre and spread	10	(0.090002, 1.166593, 5.978660)	8.62553491
WF centre and spread	11	(0.030349, -0.014548, 4.316195)	4.44936597
WF centre and spread	12	(0.000182, 1.447926, 4.202857)	0.59268107
WF centre and spread	13	(-0.000698, 1.444494, 4.201312)	0.51763118
WF centre and spread	14	(0.000123, 1.445322, 4.200517)	0.51547017
WF centre and spread	15	(-0.001147, 1.485130, 4.216010)	0.57126626
WF centre and spread	16	(-0.002077, 1.412665, 4.215952)	0.56079120
WF centre and spread	17	(1.268484, 0.337907, 8.125625)	4.57909767
WF centre and spread	18	(1.222238, 1.113089, 8.102880)	3.91815673
WF centre and spread	19	(1.253481, 0.720936, 6.145702)	0.59776856
WF centre and spread	20	(1.253559, 0.727568, 6.166295)	0.53799255
WF centre and spread	21	(1.253644, 0.719767, 6.160742)	0.52551050

WF centre and spread	22	(1.251363, 0.759526, 6.169418)	0.54149032
WF centre and spread	23	(1.248734, 0.673584, 6.169286)	0.66642573
WF centre and spread	24	(1.253189, 0.722107, 8.184431)	1.10646096
WF centre and spread	25	(0.000558, -0.001149, 8.226856)	1.04795093
WF centre and spread	26	(2.379891, 0.511930, 1.794483)	7.55948264
WF centre and spread	27	(1.052221, -0.370109, 1.787848)	7.27117180
WF centre and spread	28	(1.252999, 0.727484, 2.253193)	0.62445050
WF centre and spread	29	(1.250661, 0.731221, 2.332595)	0.64008062
WF centre and spread	30	(1.254651, 0.707306, 2.331477)	0.66426346
WF centre and spread	31	(1.253046, 0.789714, 2.292985)	0.76554890
WF centre and spread	32	(1.261775, 0.675532, 2.296954)	0.73211422
WF centre and spread	33	(-0.606168, 3.110450, 5.853896)	8.70931221
WF centre and spread	34	(0.051765, 0.054781, 4.323877)	4.97888823
WF centre and spread	35	(0.000439, 1.449217, 4.197667)	0.67442469
WF centre and spread	36	(0.000269, 1.439790, 4.200289)	0.63414148
WF centre and spread	37	(0.000425, 1.447713, 4.201899)	0.62474958
WF centre and spread	38	(-0.001409, 1.493502, 4.217393)	0.65068224
WF centre and spread	39	(-0.005369, 1.386368, 4.221517)	0.71812078
WF centre and spread	40	(1.229848, 0.350997, 8.135628)	2.42481206
WF centre and spread	41	(1.275945, 1.101073, 8.136314)	2.40703927
WF centre and spread	42	(1.261008, 0.726041, 6.133158)	0.77277954
WF centre and spread	43	(1.252222, 0.729563, 6.161395)	0.61030218
WF centre and spread	44	(1.253228, 0.717197, 6.171552)	0.59308415
WF centre and spread	45	(1.258513, 0.790886, 6.170381)	0.71080572
WF centre and spread	46	(1.267006, 0.664538, 6.171776)	0.71745759
Sum of centres and spreads	(38.105314, 41.437736, 218.986700)		94.06270572

Spreads (Ang^2) Omega I = 52.884459648

===== Omega D = 13.543379233

 Omega OD = 27.634866835

Final Spread (Ang^2) Omega Total = 94.062705715

Time for wannierise 295.212 (sec)