Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C. This journal is © The Royal Society of Chemistry 2024

Spontaneous and reversible spin-splitting in ferroelectric A-type antiferromagnetism

Liguo Zhang¹, San-Dong Guo¹ and Guangzhao Wang²
School of Electronic Engineering, Xi'an University of Posts and Telecommunications, Xi'an 710121, China and
²Key Laboratory of Extraordinary Bond Engineering and Advanced Materials Technology of Chongqing,
School of Electronic Information Engineering, Yangtze Normal University, Chongqing 408100, China

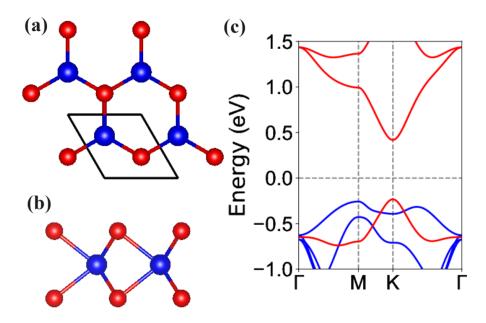


FIG. S1. (Color online) The crystal structures [top (a) and side (b) views] and energy band structures (c) of RuBr₂ monolayer. In (a) and (c), the red and blue balls represent the Br and Ru atoms, respectively. In (c), the spin-up and spin-down channels are depicted in blue and red.

```
AB-bilayer
  1.000000000000000
    3.7201954241226112
                       0.00000000000000000
                                          0.00000000000000000
    -1.8600977120613065
                       3.2217837443291479
                                          0.0000000000000000
    0.0000000000000000
                       0.0000000000000000
                                         30.6650009154999985
  Ru
       Br
    2
Direct
 0.3333333510000003
                  0.6666667029999971
                                    0.3360424894657825
 0.6666667080000011
                   0.3333333510000003
                                    0.5518023240120229
 0.6666667080000011
                   0.3333333510000003
                                    0.2794211628649776
 0.6666667080000011
                   0.3333333510000003
                                    0.3924082600640446
 0.0000000000000000
                   0.0000000000000000
                                    0.4954233696609478
  0.6084124249322329
          monolayer
  1.000000000000000
    3.7547373710534355
                       0.0000000000110835
                                           0.0000000000000000
   -1.8773686854584519
                       3.2516979478349852
                                          0.0000000000000000
    0.0000000000000000
                       0.0000000000000000
                                          24.6439990997000002
  Ru
       Br
    1
Direct
  0.3333329860000021 0.6666669849999991
                                    0.0000000000000000
 0.6666669849999991 0.3333329860000021
                                    0.9300872592475296
 0.6666669849999991 0.3333329860000021
                                    0.0699127407524706
```

FIG. S2. (Color online) The POSCAR of RuBr₂ bilayer and monolayer.

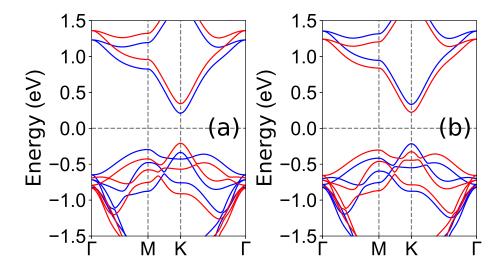


FIG. S3. (Color online) The energy band structures of AB-stacked RuBr₂ bilayer with electric field +0.10 V/Å (a) and -0.10 V/Å (b). The spin-up and spin-down channels are depicted in blue and red.

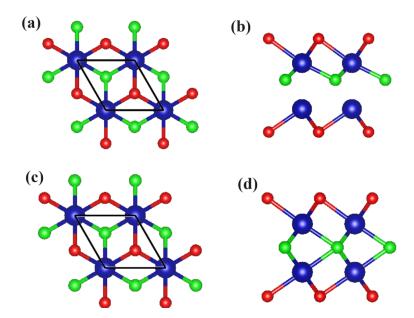


FIG. S4. (Color online) The crystal structures [top (a,c) and side (b,d) views] of Co_2CF_2 monolayer with $H^{'}$ (a,b) and H (c,d) phases. The red, blue and green balls represent the F, Co and C atoms, respectively.

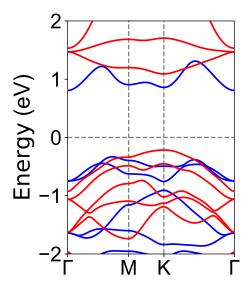


FIG. S5. (Color online) The energy band structures of Co₂CF₂ monolayer with H['] phase. The spin-up and spin-down channels are depicted in blue and red.

```
AC
   1.000000000000000
     2.8688034880388176
                           0.0000000000000000
                                                   0.0000000000000000
     -1.4344017440688628
                            2.4844566990685766
                                                   0.0000000000000000
     0.0000000000000000
                            0.00000000000000000
                                                  32.2830009460000014
             Co
Direct
                      0.6666666750000019
                                           0.5858887893138416
  0.3333333380000028
  0.0000000000000000
                      0.00000000000000000
                                           0.8111833089361653
                                           0.7306364070679621
  0.3333333380000028
                      0.6666666750000019
  0.3333333380000028
                      0.6666666750000019
                                           0.8751821804037121
  0.6666666690000014
                      0.3333333380000028
                                           0.5052370144777427
  0.6666666690000014
                      0.3333333380000028
                                           0.6501866095546376
  0.6666666690000014
                      0.3333333380000028
                                           0.7662186000198830
  0.6666666690000014
                      0.3333333380000028
                                           0.8372825761417388
  9.99999999999999
                      0.00000000000000000
                                           0.5409922390746544
  0.00000000000000000
                      0.00000000000000000
                                           0.6121823600096548
   1.000000000000000
     2.8688034880388176
                           0.0000000000000000
                                                  0.0000000000000000
    -1.4344017440688628
                           2.4844566990685766
                                                  0.00000000000000000
     0.00000000000000000
                           0.00000000000000000
                                                  32.2830009460000014
             Co
     2
Direct
  0.3333333380000028
                      0.6666666750000019
                                           0.41411000000000009
  0.0000000000000000
                      0.0000000000000000
                                           0.188819999999998
                      0.6666666750000019
                                           0.2693599999999989
  0.3333333380000028
  0.3333333380000028
                      0.6666666750000019
                                           0.1248199999999997
  0.6666666690000014
                      0.3333333380000028
                                           0.4947599999999994
  0.6666666690000014
                      0.3333333380000028
                                           0.3498099999999980
  0.6666666690000014
                      0.3333333380000028
                                           0.23378000000000030
  0.6666666690000014
                      0.3333333380000028
                                           0.16272000000000002
  0.00000000000000000
                      0.0000000000000000
                                           0.459009999999993
  0.0000000000000000
                      0.0000000000000000
                                           0.3878199999999978
```

FIG. S6. (Color online) The POSCAR of H'-Co₂CF₂ bilayer systems with AC and AB patterns.

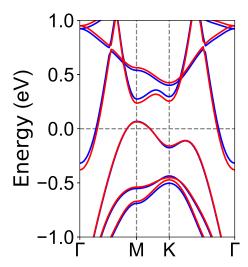


FIG. S7. (Color online) The energy band structures of bilayer Co_2CF_2 , where the C atoms of AC patter are artificially moved on the central horizontal plane of Co dimers. The spin-up and spin-down channels are depicted in blue and red.