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

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FIG. S1. (Color online) The crystal structures [top (a) and side (b) views] and energy band structures (c) of $\mathrm{RuBr}_{2}$ 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-bilayen |  |  |
| :---: | :---: | :---: |
| 1.00000000000000 |  |  |
| 3.7201954241226112 | 120.0000000000000000 | 0.0000000000000000 |
| -1.8600977120613065 | 3.2217837443291479 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 30.6650009154999985 |
| Ru Br |  |  |
|  |  |  |
| Direct |  |  |
| 0.33333335100000030 | 0.66666670299999710 .3 | 0424894657825 |
| 0.6666667080000011 | 0.33333335100000030 .5 | 8023240120229 |
| 0.6666667080000011 | 0.33333335100000030 .2 | 4211628649776 |
| 0.66666670800000110 | 0.33333335100000030 .3 | 4082600640446 |
| 0.0000000000000000 0 | 0.00000000000000000 .49 | 4233696609478 |
| 0.0000000000000000 | 0.0000000000000000 0.60 | 4124249322329 |
| 'monolayer |  |  |
| 1.00000000000000 |  |  |
| 3.7547373710534355 | 550.0000000000110835 | 0.0000000000000000 |
| -1.8773686854584519 | 3.2516979478349852 | 0.0000000000000000 |
| 0.000000000000000 | 0.0000000000000000 | 24.6439990997000002 |
| Ru Br |  |  |
|  |  |  |
| Direct |  |  |
| 0.33333298600000210 | 0.66666698499999910 .0 | 0000000000000 |
| 0.6666669849999991 | 0.33333298600000210 .9 | 0872592475296 |
| 0.6666669849999991 | 0.33333298600000210 .0 | 9127407524706 |

FIG. S2. (Color online) The POSCAR of $\mathrm{RuBr}_{2}$ bilayer and monolayer.


FIG. S3. (Color online) The energy band structures of $A B-$ stacked $\mathrm{RuBr}_{2}$ bilayer with electric field $+0.10 \mathrm{~V} / \AA$ (a) and -0.10 $\mathrm{V} / \AA(\mathrm{b})$. The spin-up and spin-down channels are depicted in blue and red.

(b)



(d)


FIG. S4. (Color online) The crystal structures [top ( $\mathrm{a}, \mathrm{c}$ ) and side ( $\mathrm{b}, \mathrm{d}$ ) views] of $\mathrm{Co}_{2} \mathrm{CF}_{2}$ monolayer with $\mathrm{H}^{\prime}(\mathrm{a}, \mathrm{b})$ and $\mathrm{H}(\mathrm{c}, \mathrm{d})$ phases. The red, blue and green balls represent the F, Co and C atoms, respectively.


FIG. S5. (Color online) The energy band structures of $\mathrm{Co}_{2} \mathrm{CF}_{2}$ monolayer with $\mathrm{H}^{\prime}$ phase. The spin-up and spin-down channels are depicted in blue and red.
AC
1.00000000000000

| 2.8688034880388176 | 0.0000000000000000 | 0.0000000000000000 |
| ---: | ---: | ---: |
| -1.4344017440688628 | 2.4844566990685766 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 32.2830009460000014 |

$\mathrm{C}_{2} \mathrm{~F}_{4}^{\mathrm{Co}}$
Direct
$0.3333333380000028 \quad 0.6666666750000019 \quad 0.5858887893138416$
0.3333333380000028 0.0000000000000000
0.8111833089361653
0.7306364070679621
0.8751821804037121
 0.6666666750000019 0.5052370144777427
0.6501866095546376
0.6666666690000014 0.3333333380000028
0.7662186000198830
0.6666666690000014
0.3333333380000028
0.8372825761417388
0.000000000000000
$0.0000000000000000 \quad 0.5409922390746544$
$0.0000000000000000 \quad 0.0000000000000000 \quad 0.6121823600096548$
AB
1.00000000000000

| 2.8688034880388176 | 0.0000000000000000 | 0.0000000000000000 |
| ---: | ---: | ---: |
| -1.4344017440688628 | 2.4844566990685766 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 32.2830009460000014 |

C
Co
$2 \quad 4 \quad 4$
Direct
$0.3333333380000028 \quad 0.6666666750000019 \quad 0.4141100000000009$
$0.0000000000000000 \quad 0.000000000000000 \quad 0.1888199999999998$
$0.3333333380000028 \quad 0.6666666750000019 \quad 0.2693599999999989$
$0.3333333380000028 \quad 0.6666666750000019 \quad 0.1248199999999997$
$0.66666666900000140 .3333333380000028 \quad 0.4947599999999994$
0.6666666690000014
0.33333333800000280 .3498099999999980
$\begin{array}{llll}0.6666666690000014 & 0.3333333380000028 & 0.2337800000000030 \\ 0.6666666690000014 & 0.3333333380000028 & 0.1627200000000002\end{array}$
$0.0000000000000000 \quad 0.0000000000000000 \quad 0.4590099999999993$
$0.0000000000000000 \quad 0.00000000000000000 .3878199999999978$

FIG. S6. (Color online) The POSCAR of $\mathrm{H}^{\prime}-\mathrm{Co}_{2} \mathrm{CF}_{2}$ bilayer systems with AC and AB patterns.


FIG. S7. (Color online) The energy band structures of bilayer $\mathrm{Co}_{2} \mathrm{CF}_{2}$, 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.

