Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Pure spin currents induced by asymmetric H-passivation in $B_3C_2P_3$ nanoribbons

Table. S1 Total energy of all structures under NFM, FM and AFM states

type	E_{total}		
	NFM	FM	AFM
zB_P	-124.4876	-124.4896	-124.4896
zB_CP	-101.4310	-101.4350	-101.4345
zCB_P	-105.9040	-105.9113	-105.9111
zCB_CP	-82.8606	-82.8602	-82.8606
1H-zB_P-0H	-125.6932	-125.7047	-125.7056
1H-zB_CP-0H	-102.7210	-102.7320	-102.7326
1H-zCB_P-0H	-107.1164	-107.1318	-107.1312
1H-zCB_CP-0H	-84.1392	-84.1483	-84.1487
2H-zB_P-0H	-126.8822	-126.8842	-126.8830
2H-zB_CP-0H	-103.8944	-103.8995	-103.8967
2H-zCB_P-0H	-108.3056	-108.3195	-108.3203
2H-zCB_CP-0H	-85.3159	-85.3333	-85.3326
0H-zB_P-1H	-125.8157	-125.8158	-125.8185
0H-zB_CP-1H	-102.7605	-102.7659	-102.7648
0H-zCB_P-1H	-107.2428	-107.2426	-107.2430
0H-zCB_CP-1H	-84.1868	-84.1897	-84.1896
0H-zB_P-2H	-126.9601	-126.9632	-126.9642
0H-zB_CP-2H	-103.9046	-103.9090	-103.9084
0H-zCB_P-2H	-108.4150	-108.4185	-108.4173
0H-zCB_CP-2H	-85.3564	-85.3663	-85.3618
1H-zB_P-1H	-127.0585	-127.0557	-127.0571
1H-zB_CP-1H	-104.0497	-104.0529	-104.0534
1H-zCB_P-1H	-108.4687	-108.4681	-108.4712
1H-zCB_CP-1H	-85.4773	-85.4795	-85.4793
2H-zB_P-1H	-128.2247	-128.2214	-128.2239
2H-zB_CP-1H	-105.2356	-105.2389	-105.2377
2H-zCB_P-1H	-109.6405	-109.6401	-109.6439
2H-zCB_CP-1H	-86.6560	-86.6565	-86.6559
1H-zB_P-2H	-128.2017	-128.1987	-128.2021
1H-zB_CP-2H	-105.1932	-105.1992	-105.1992
1H-zCB_P-2H	-109.6539	-109.6561	-109.6565
1H-zCB_CP-2H	-86.6432	-86.6529	-86.6480
2H-zB_P-2H	-129.3675	-129.3667	-129.3718
2H-zB_CP-2H	-106.3837	-106.3813	-106.3840
2H-zCB_P-2H	-110.8154	-110.8213	-110.8209
2H-zCB_CP-2H	-87.8573	-87.8566	-87.8550

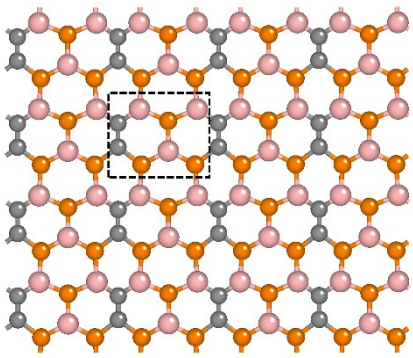

Fig. S1 The two-dimensional $B_3C_2P_3$ material (black dashed line represents its primitive cell).

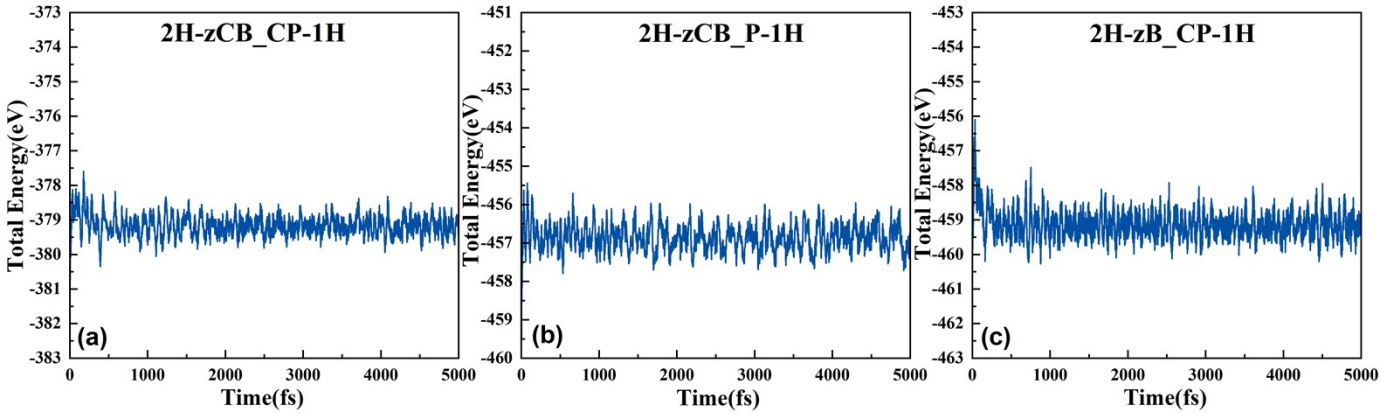

Fig. S2 Variations of the total energy of (a) 2H-zCB_CP-1H (b) 2H-zCB_P-1H (c) 2H-zB_CP-1H at 300 K during AIMD simulations.