Electronic Supplementary Material (ESI) for RSC Advances.

Spin Filtering Controller Induced by Phase Transitions in Fluorographane

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Table S1 The blochstates of the VBM and CBM at Γ for B-C_2HF nanoribbons with FM and AFM state.

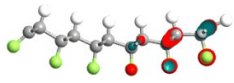
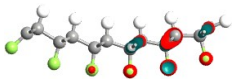
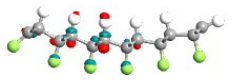
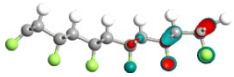
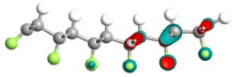
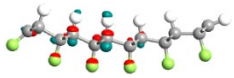
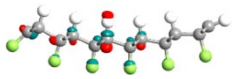
	VBM-C_2HF		CBM-C_2HF	
	down	up	down	up
B-C_2HF-zigzag-FM				
B-C_2HF-zigzag-AFM				

Table S2 The blochstates of the VBM and CBM at Γ for the H-C_2HF-zigzag and B-C_2HF-armchair and H-C_2HF-armchair nanoribbons.

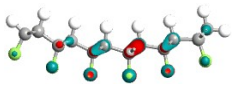
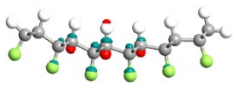
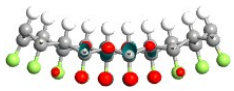
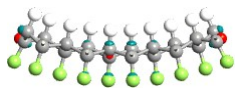
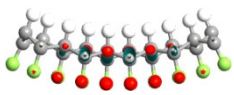
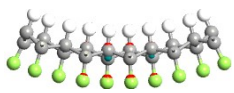
	VBM-C_2HF	CBM-C_2HF
H-C_2HF-zigzag		
B-C_2HF-armchair		
H-C_2HF-armchair		

Table S3 The Mulliken population of the edge C atoms in B-C_2HF-armchair nanoribbons

Element		C	C	C	C	C	C	C	C	C	C
Mulliken Population	Spin-up	2.04	1.99	1.99	1.98	1.96	1.99	1.98	1.97	1.97	1.95
	Spin-down	2.04	1.99	1.99	1.98	1.96	1.99	1.98	1.97	1.97	1.95
Element		C	C	C	C	C	C	C	C	C	C
Mulliken Population	Spin-up	1.96	1.98	1.98	1.99	2.04	1.95	1.97	1.97	1.98	1.99
	Spin-down	1.96	1.98	1.98	1.99	2.04	1.95	1.97	1.97	1.98	1.99
Element		H	H	H	H	H	H	H	H	H	H
Mulliken Population	Spin-up	0.53	0.53	0.53	0.53	0.52	0.52	0.53	0.53	0.53	0.53
	Spin-down	0.53	0.53	0.53	0.53	0.52	0.52	0.53	0.53	0.53	0.53
Element		F	F	F	F	F	F	F	F	F	F
Mulliken Population	Spin-up	3.47	3.52	3.51	3.51	3.52	3.52	3.51	3.51	3.52	3.47
	Spin-down	3.47	3.52	3.51	3.51	3.52	3.52	3.51	3.51	3.52	3.47

Table S4 The Mulliken population of the edge C atoms in B-C_2HF-zigzag nanoribbons.

Element		C	C	C	C	C	C	C	C	C	C	C	C
Mulliken Population	Spin-up	1.98	1.98	1.99	1.92	1.97	1.91	1.99	1.99	2.42	1.67	1.97	1.97
	Spin-down	1.95	1.99	1.98	2.03	1.97	1.92	1.99	1.99	1.61	3.37	1.97	1.97
Element		H	H	H	H	H	H	F	F	F	F	F	F
Mulliken Population	Spin-up	0.51	0.53	0.53	0.53	0.53	0.52	3.51	3.52	3.62	3.42	3.52	3.51
	Spin-down	0.54	0.53	0.53	0.53	0.53	0.53	3.51	3.52	3.48	3.52	3.52	3.51

Table S5 Calculation magnetic moments for the edge C of B-C_2HF-zigzag nanoribbon

Species	C_8-AFM	C_9-AFM	C_8-FM	C_9-FM
Magnetic Moment, S (μB)	0.90	-0.84	0.90	0.84