Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information

Investigation of doping effects on magnetic properties of the hydrogenated and fluorinated graphene structures by extra charge mimic

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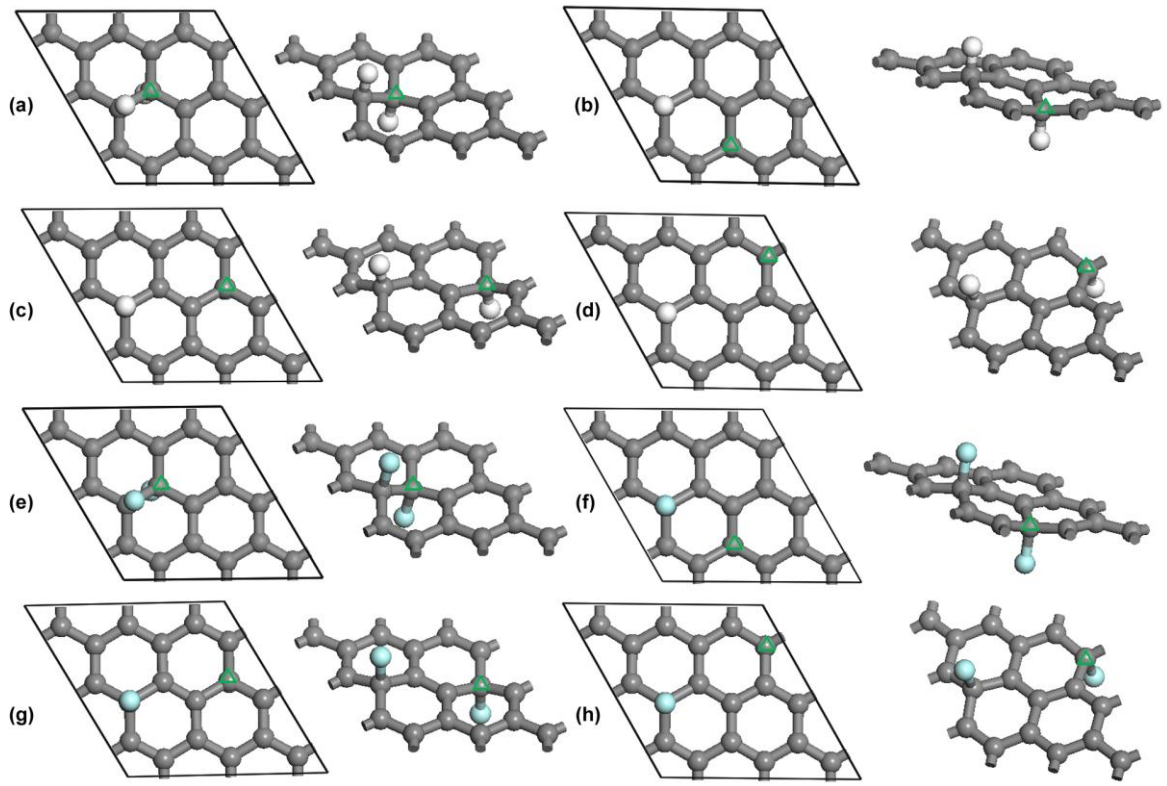
Table S 1 The up- and down-spin Milliken charges, spin moments, and the bond length between carbon and hydrogen atoms of the hydrogenated graphene with different extra charges to mimic the doping effects.

Charged (*e*)	Mulliken (*e*) (spin up)	Mulliken (*e*) (spin down)	Mulliken (*e*) (up+down)	Spin Moment (μ_B) (up-down)	C_α-H (Å)
-1	38.000	37.000	75.000	1.000	1.147
-0.9	38.000	36.900	74.900	1.100	1.146
-0.8	38.000	36.800	74.800	1.200	1.144
-0.7	38.000	36.700	74.700	1.300	1.144
-0.6	38.000	36.600	74.600	1.400	1.143
-0.5	38.000	36.500	74.500	1.500	1.142
-0.4	38.000	36.400	74.400	1.600	1.141
-0.3	38.000	36.300	74.300	1.700	1.140
-0.2	38.000	36.200	74.200	1.800	1.140
-0.1	38.000	36.100	74.100	1.900	1.139
0	37.999	36.001	74.000	1.998	1.141
0.1	37.900	36.000	73.900	1.900	1.142
0.2	37.800	36.000	73.800	1.800	1.140
0.3	37.700	36.000	73.700	1.700	1.141
0.4	37.600	36.000	73.600	1.600	1.141
0.5	37.500	36.000	73.500	1.500	1.142
0.6	37.400	36.000	73.400	1.400	1.143
0.7	37.299	36.001	73.300	1.298	1.143
0.8	37.199	36.001	73.200	1.198	1.144
0.9	37.099	36.001	73.100	1.098	1.145
1.0	36.999	36.001	73.000	0.998	1.146

Table S 2 The up- and down-spin Milliken charges, spin moments, and the bond length between carbon and fluorine atoms of the fluorinated graphene with different extra charges to mimic the doping effects.

Charged (*e*)	Mulliken (*e*) (spin up)	Mulliken (*e*) (spin down)	Mulliken (*e*) (up+down)	Spin Moment (μ_B) (up-down)	C_α-F (Å)
-1	-	-	87.000	-	1.528
-0.9	-	-	86.900	-	1.519
-0.8	-	-	86.800	-	1.510
-0.7	-	-	86.700	-	1.503
-0.6	-	-	86.600	-	1.496
-0.5	43.465	43.035	86.500	0.430	1.489
-0.4	43.484	42.916	86.400	0.568	1.482
-0.3	43.477	42.823	86.300	0.654	1.475
-0.2	43.447	42.753	86.200	0.694	1.468
-0.1	43.408	42.692	86.100	0.716	1.461
0	43.361	42.639	86.000	0.722	1.456
0.1	43.335	42.565	85.900	0.770	1.450
0.2	43.318	42.482	85.800	0.836	1.445
0.3	43.310	42.390	85.700	0.920	1.441
0.4	43.302	42.298	85.600	1.004	1.437
0.5	43.276	42.224	85.500	1.052	1.434
0.6	43.244	42.156	85.400	1.088	1.430
0.7	43.183	42.117	85.300	1.066	1.426
0.8	43.118	42.082	85.200	1.036	1.423
0.9	43.026	42.074	85.100	0.952	1.420
1.0	42.929	42.071	85.000	0.858	1.418



5 Figure S 1 Other configurations of these two adatoms. Carbon, fluorine, and hydrogen atoms are colored in grey, cyan and white, respectively. The green triangles display the unseen connections between carbon atoms and groups on the back side.

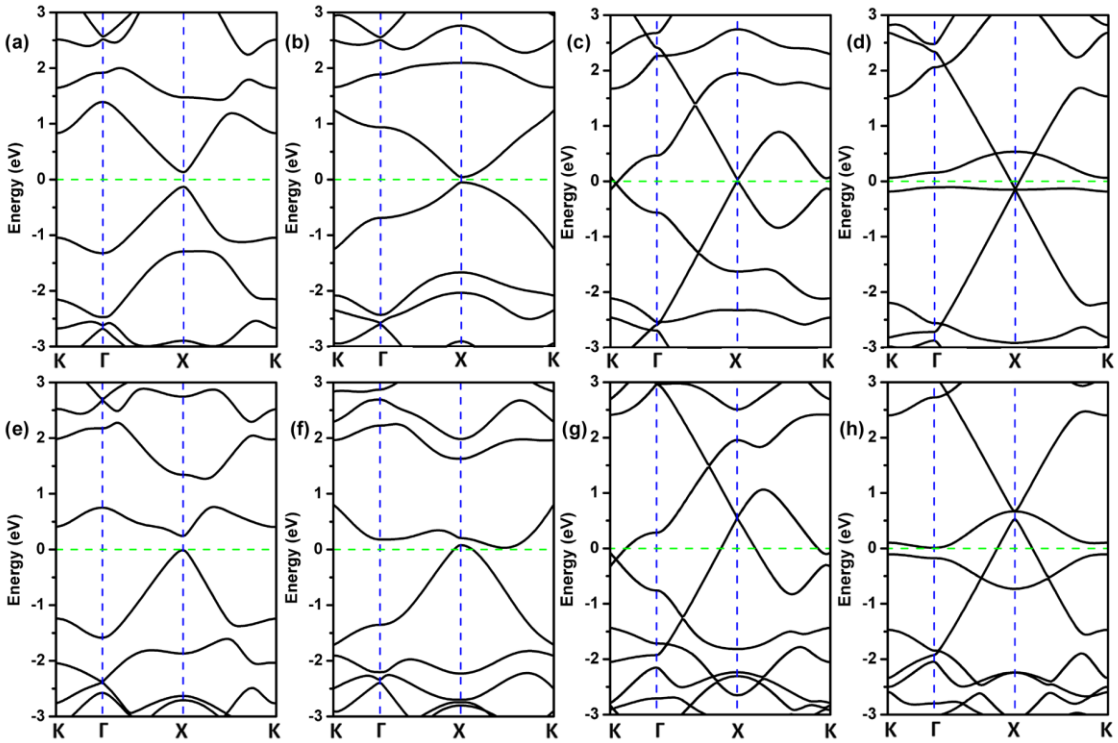


Figure S 2 Band structures of the (a)-(d) hydrogenated and (e)-(h) fluorinated graphenes. K ($2\pi/3a$, $2\pi/3a$, 0), X (0, π/a, 0), and Γ (0, 0, 0). The Fermi level, denoted as green dashed line, is set to zero.