Supporting Information

Electronic structure engineering via on-plane chemical functionalization: A comparison study on two-dimensional polysilane and graphane

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Table S1. Energies (in eV) of fluorinated gaphane (C-F) and polysilane (Si-F) in different configurations.

	25-a	25-b	25-c	50-a	50-b	50-c	50-d	50-e	50-f	75-a	75-b	75-c	100
C-F	-103.12	-103.48	-103.57	-102.11	-103.34	-103.53	-103.44	-103.02	-103.13	-102.39	-102.63	-102.74	-101.29
Si-F	-74.18	-74.19	-74.22	-78.00	-78.03	-78.11	-78.07	-78.03	-78.07	-81.80	-81.80	-81.85	-85.41

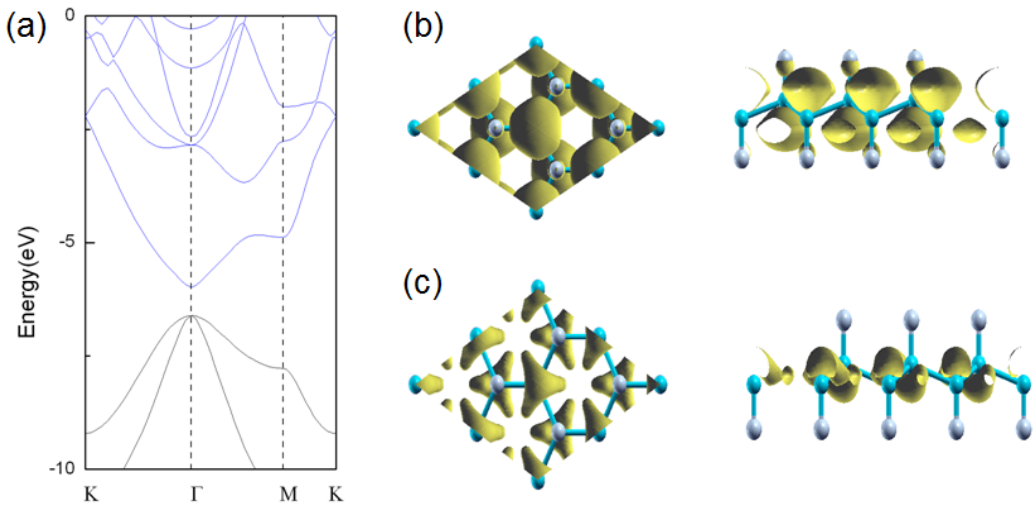

Figure S1. (a) Band structure of the 100% fluorinated polysilane using a 1×1 unit cell. Density of CBM at (b) the Γ point and (c) the M point.

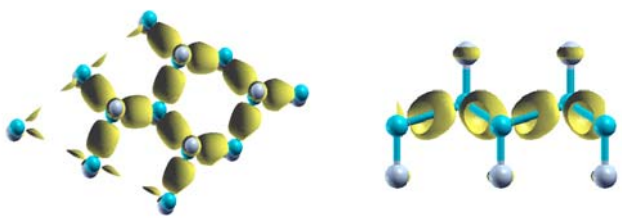

Figure S2. Density of VBM for 100% fluorinated planar polysilane.

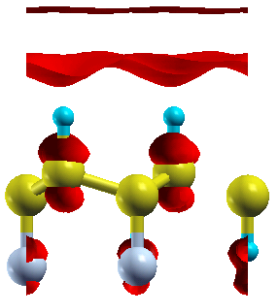

Figure S3. Density of CBM of fluorinated graphane (configuration 25-a).

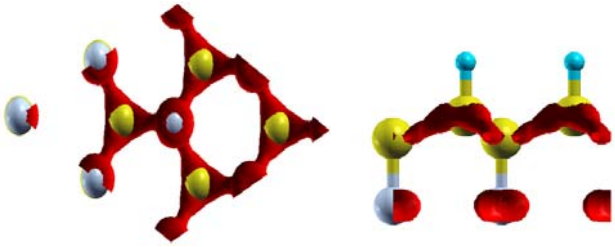

Figure S4. Density of VBM of fluorinated graphane (configuration 50-a).

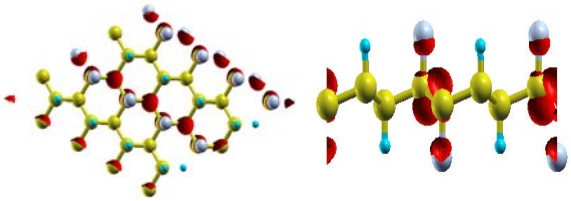

Figure S5. Density of CBM of fluorinated graphane (configuration 50-b).

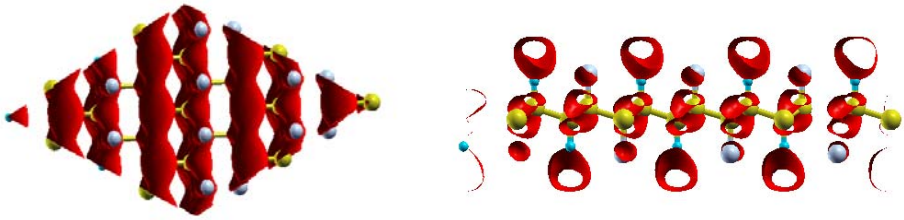

Figure S6. Density of conduction band edge (CBE) at the Γ point of 50% fluorinated graphane (configuration 50-c).

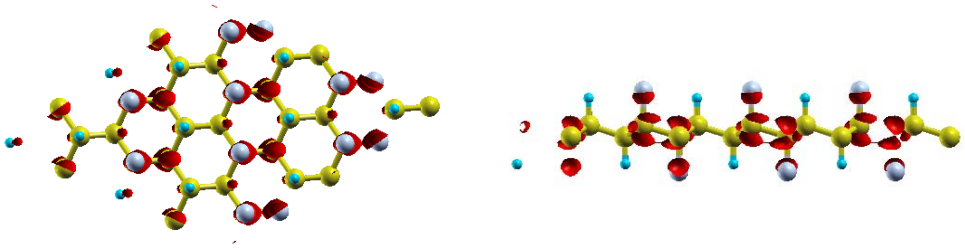

Figure S7. Density of CBM at the k-point between Γ and M for the 50% fluorinated graphane (configuration 50-c).

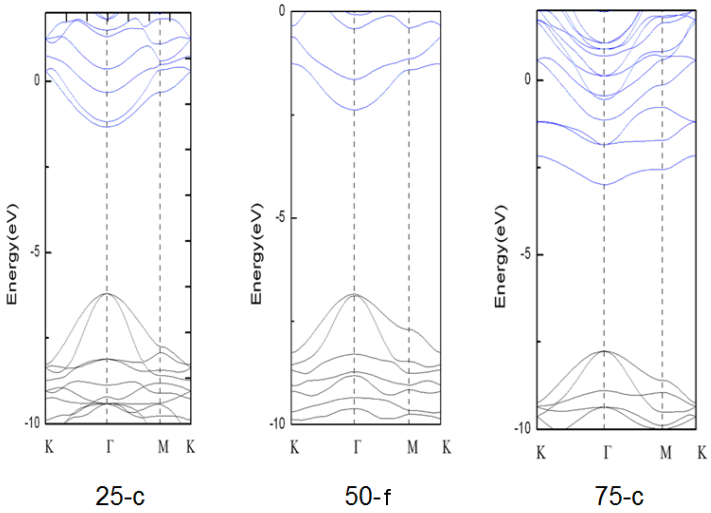

Figure S8. Band structure of 25-c, 50-f, 75-c fluorinated graphane from left to right respectively.

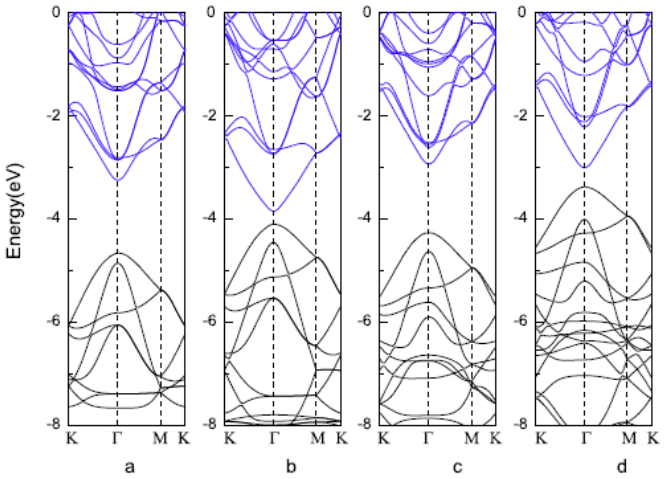

Figure S9. Band structure of (a) 50% and (b) 100% OH covered or (c)50% and (d) 100% NH_2 covered planar polysilane.

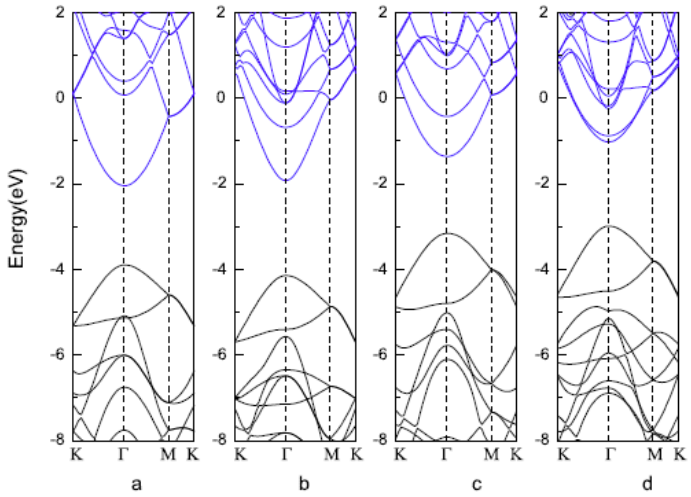

Figure S10. Band structure of (a) 50% and (b) 100% OH covered or (c) 50% and (d) 100% NH_2 covered graphane.

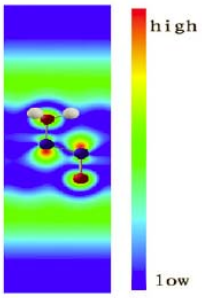

Figure S11. CBM density in 100% NH_2 covered graphane.