**Supporting information for**

# Redox reactions between acetonitrile and nitrogen dioxide in interlayer space of fluorinated graphite matrices

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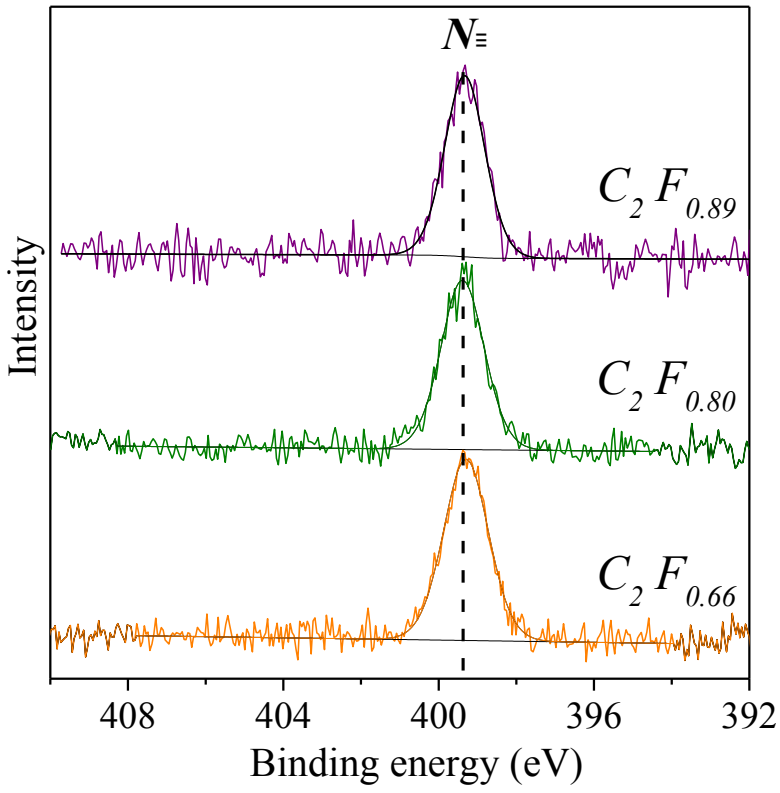


Fig. S1. XPS N 1s-spectra of fluorinated graphite intercalation compounds (FGICs) based on various $C_2F_x$ matrices with acetonitrile.

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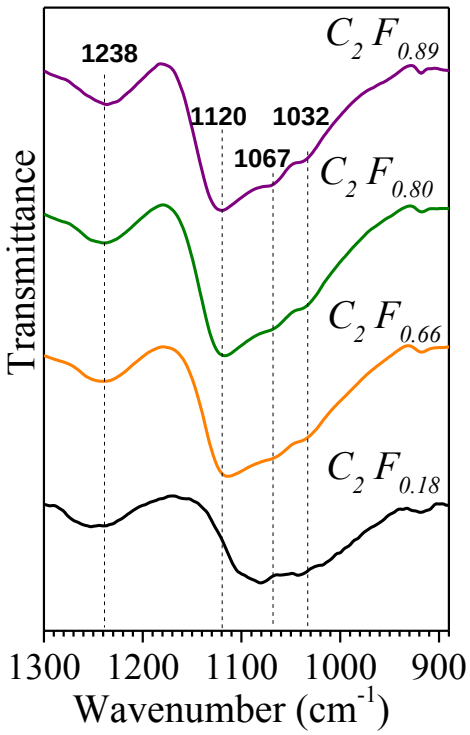


Fig. S2. C–F vibration region of IR-spectra of FGICs based on various $C_2F_x$ matrices with acetonitrile. Bold numbers from lowest to highest identify frequencies of the stretching vibrations for isolated CF groups and CF groups with two, one, and no bare carbon neighbors, respectively.

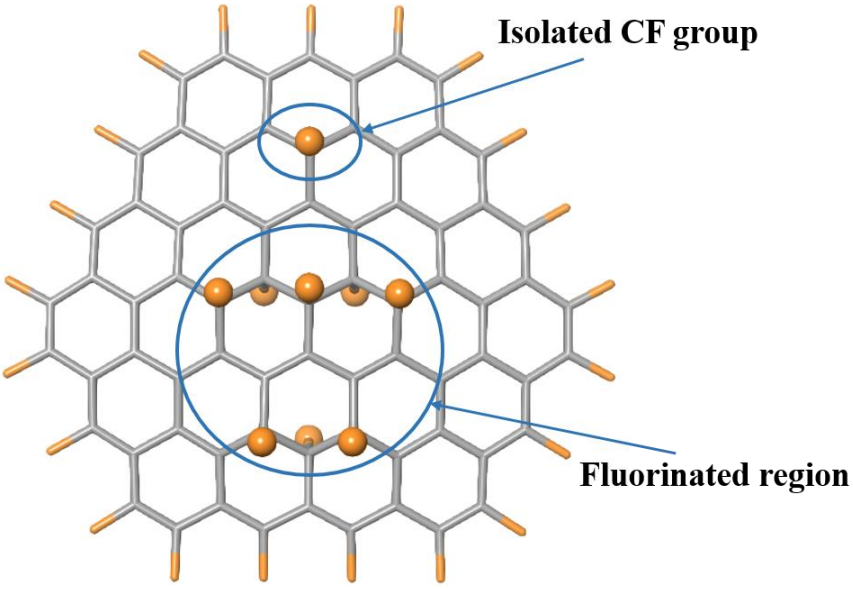


Fig. S3. Model of partially fluorinated graphene layer with isolated CF group and fluorinated region of zigzag CF chains separated by bare carbon atoms. The fragment edges are terminated by fluorine atoms.

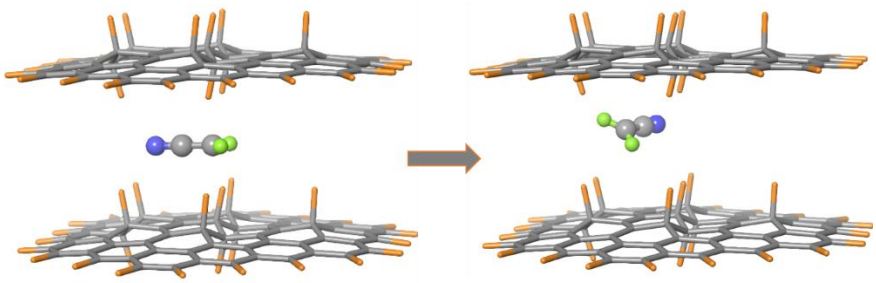

Fig. S4. Model of partially fluorinated graphene bilayer intercalated with $CH_2CN$. Left – starting position of $CH_2CN$ between fluorinated regions of the layers. Right – the structure of model optimized at B3LYP/6-31G. $CH_2CN$ rotated and located over $sp^2$-hybridized carbon chains in the gallery of fluorinated graphene bilayer.