

Supplementary Information File

Functionalised Biphenylene and Graphenylene: Excellent Choices for Supercapacitor Electrode

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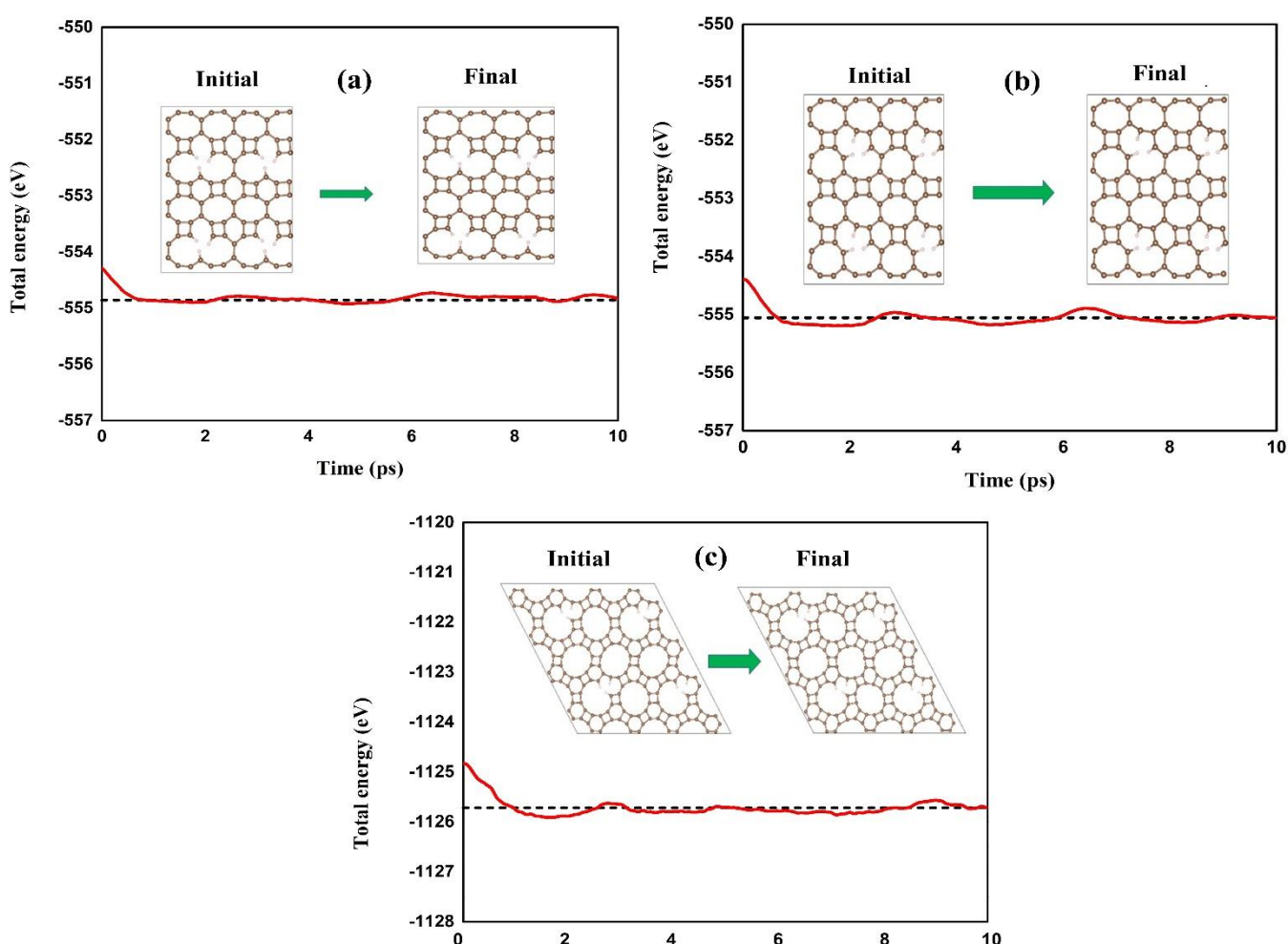
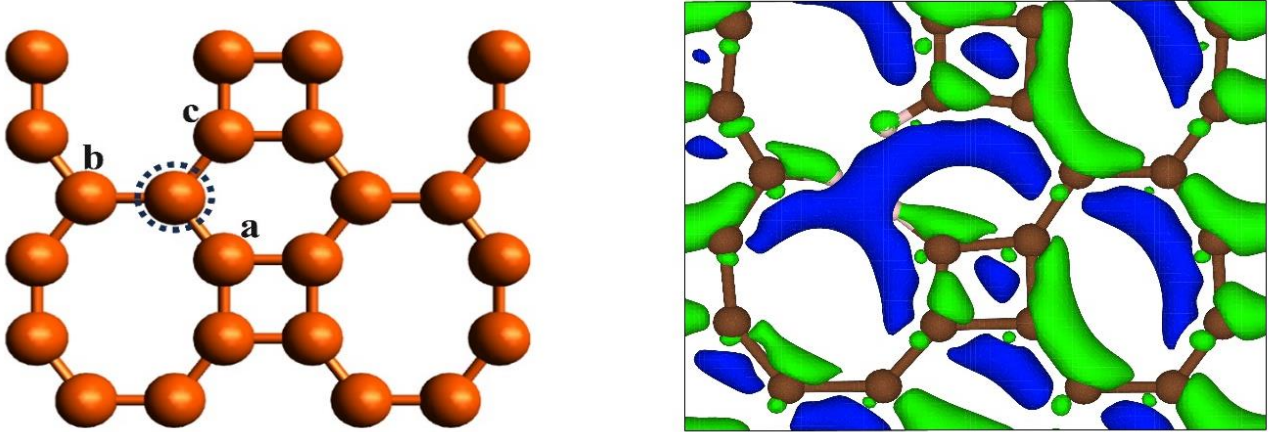


Fig.S1: Total energy vs time plot of (a) BPN (Vacancy 1), (b) BPN (Vacancy 2), (c) GPN (Vacancy 1) obtained from AIMD simulation at 300 K.

(a)



(b)

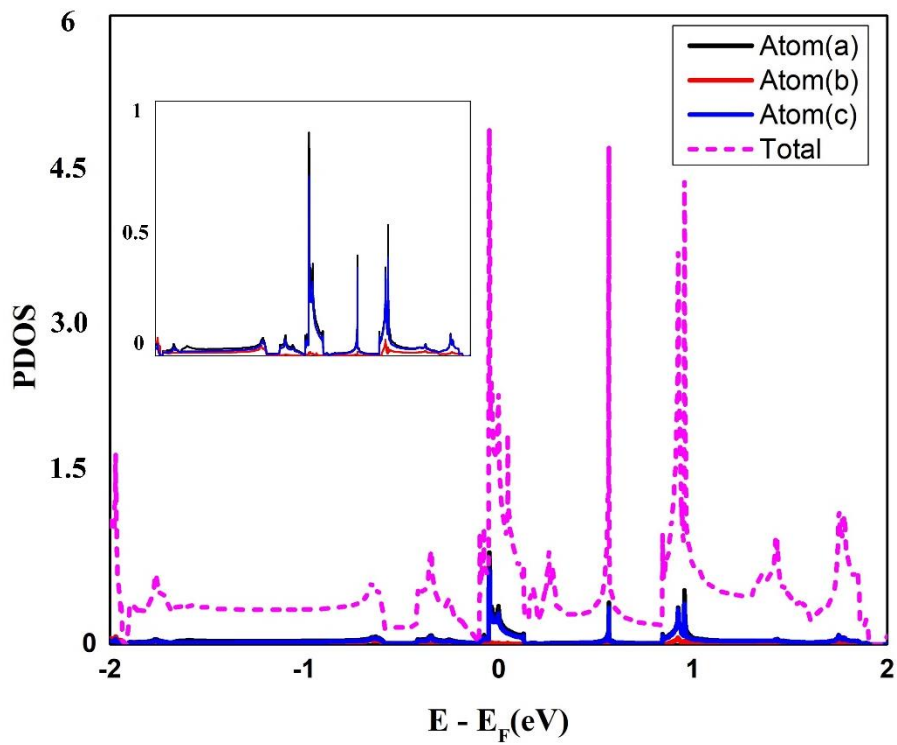


Fig.S2: (a) Vacancy modified BPN monolayer (vacancy 1) and corresponding charge density difference plot. The green and blue color denote accumulation and depletion of charges. The isosurface value is set to $0.05 \text{ e}/\text{\AA}^3$ (b) PDOS analysis of vacancy modified defective BPN monolayers. The contribution of p orbital of individual atoms is shown in the inset.

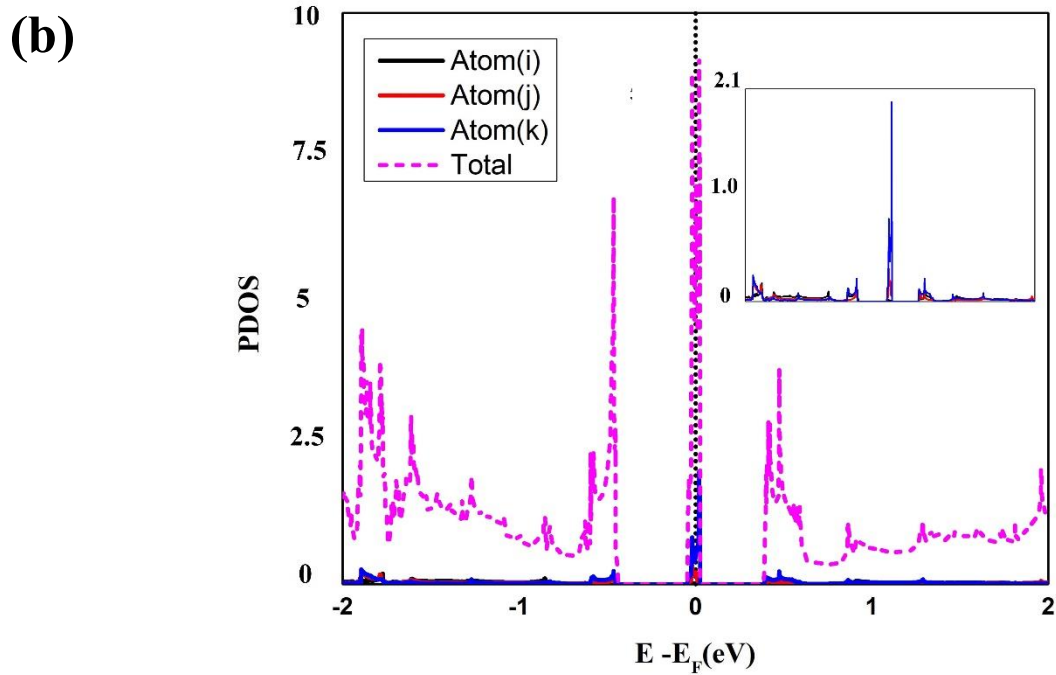
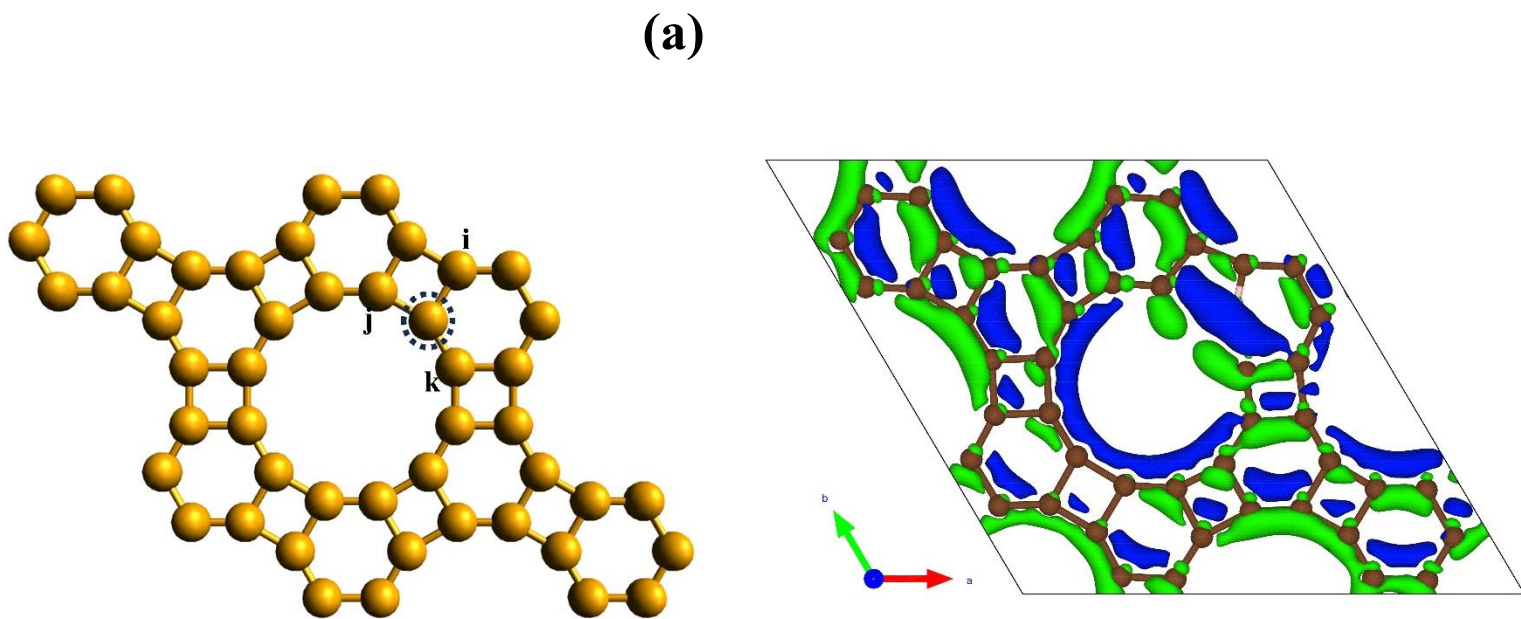


Fig.S3: (a) Vacancy modified GPN monolayer and corresponding charge density difference plot. The green and blue color denote accumulation and depletion of charges. The isosurface value is set to $0.07 \text{ e}/\text{\AA}^3$ (b) PDOS analysis of vacancy modified defective GPN monolayers. The contribution of p orbital of individual atoms is shown in the inset.