

## Supporting Information

### Computational Investigation of Formaldehyde Adsorption on Nitrogen-Doped- $\gamma$ -Graphyne: Modulation by External Electric Field and Mechanical Strain

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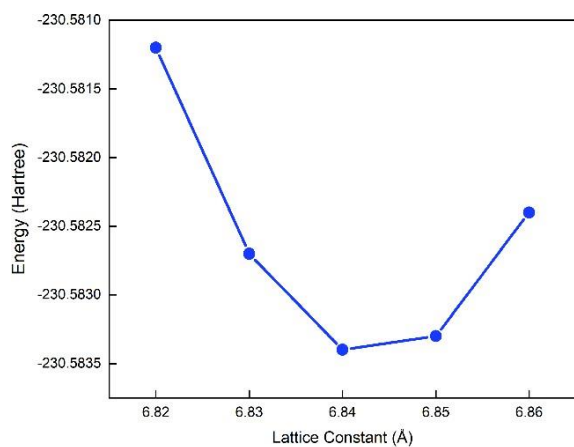
Email: [msarma@iitg.ac.in](mailto:msarma@iitg.ac.in)

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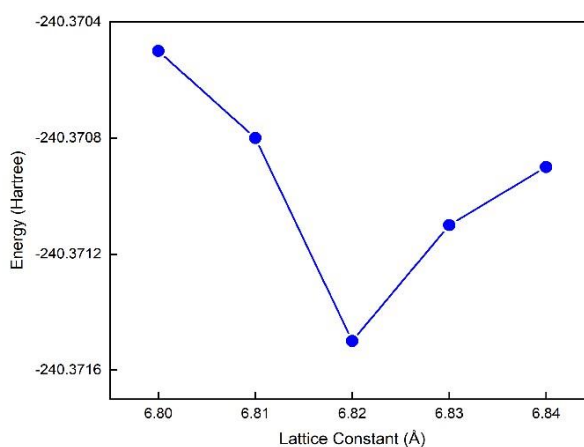
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**Table S1:** Benchmark of structural and electronic properties of pristine  $\gamma$ -graphyne.

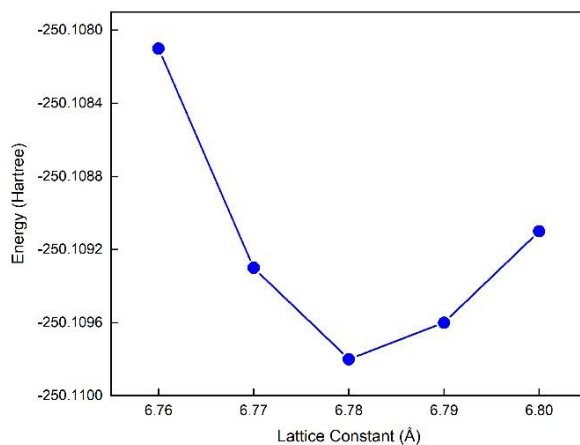
Parameters	Our Results	Previous Results
Lattice Constant	6.89 Å	6.89 Å [1]
Electronic band gap	0.42 eV (Direct)	0.46 eV (Direct) [1]
Work function	4.99 eV	5.17 eV [2]



(a)

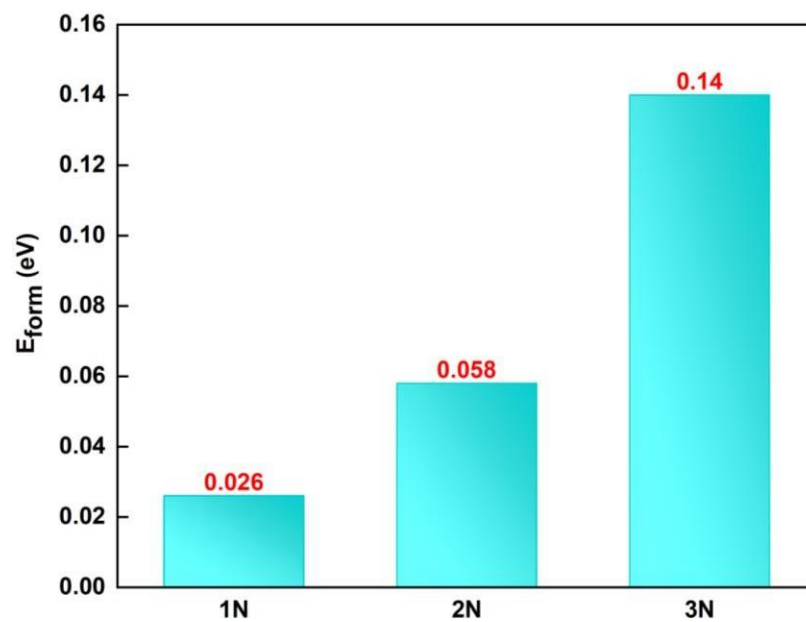


(b)

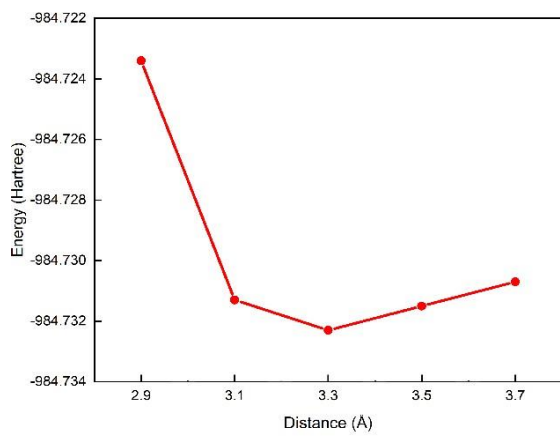


(c)

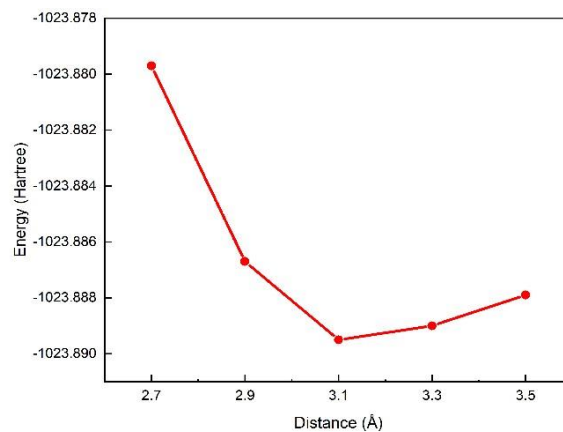
**Figure S1:** Lattice constant (LA) plots of (a) 1N- $\gamma$ -graphyne, (b) 2N- $\gamma$ -graphyne, and (c) 3N- $\gamma$ -graphyne.



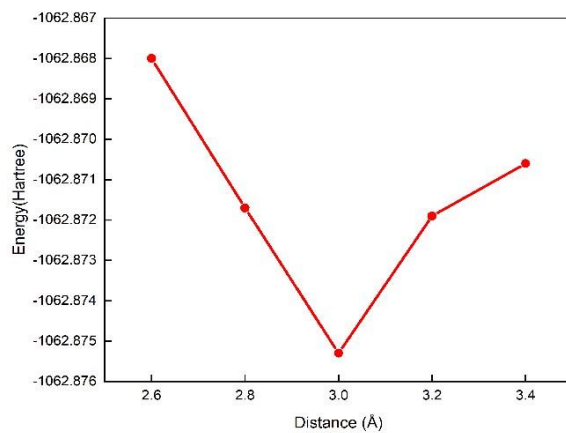
**Figure S2:** Formation energy ( $E_{form}$ ) plots of the N-doped- $\gamma$ -graphyne system having different nitrogen doping concentrations.



(a)

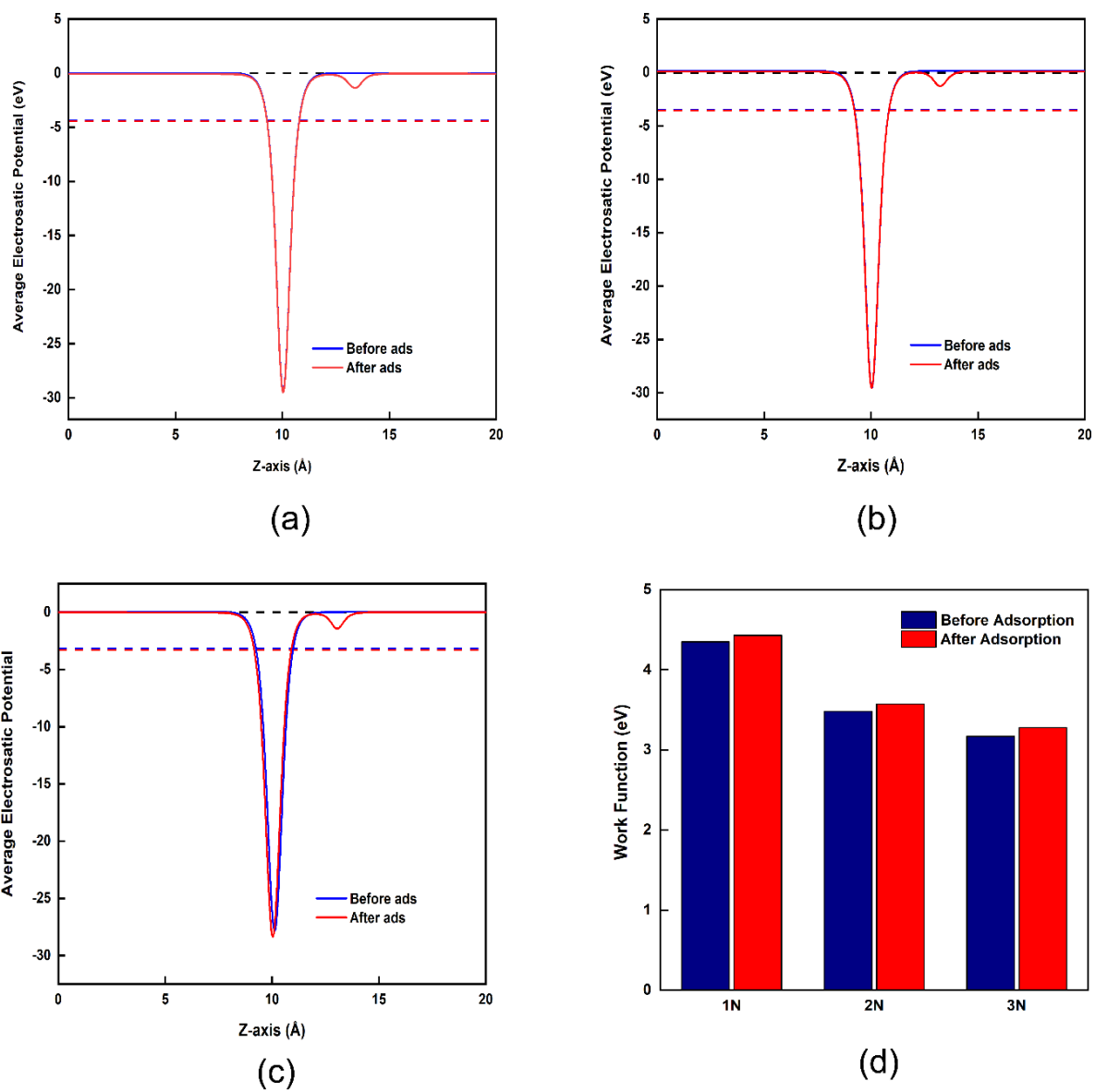


(b)



(c)

**Figure S3:** Potential Energy Curves (PECs) of (a) 1N- $\gamma$ -graphyne, (b) 2N- $\gamma$ -graphyne, and (c) 3N- $\gamma$ -graphyne.



**Figure S4:** Average Electrostatic Potential plots of (a) 1N- $\gamma$ -graphyne, (b) 2N- $\gamma$ -graphyne, (c) 3N- $\gamma$ -graphyne, and (d) Work function ( $\phi$ ) plots before and after adsorption of  $\text{H}_2\text{CO}$  molecule.

## **References**

1. A. Ruiz-Puigdollers and P. Gamallo, *Carbon*, 2017, **114**, 301-310.
2. X. Deng, J. Zeng, M. Si, and W. Lu, *Europhys. Lett.*, 2016, **115**, 27009 (p1-p6).