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Correction: DFT investigation of the oxygen reduction reaction over nitrogen (N) doped graphdiyne as an electrocatalyst: the importance of pre-adsorbed OH* and the solvation effect

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Correction for 'DFT investigation of the oxygen reduction reaction over nitrogen (N) doped graphdiyne as an electrocatalyst: the importance of pre-adsorbed OH* and the solvation effect' by Yuelin Wang *et al.*, *Mater. Adv.*, 2023, <https://doi.org/10.1039/d3ma00502j>.

The authors regret that on the 5th page of the article, in the three paragraphs from “Consequently, upon applying a limiting potential of 0.22 V...” to “...cannot be used as an ORR electrocatalyst.”, all instances of ‘sp-N1GDY(OH)/GDY’ and ‘sp-N2GDY(OH)/GDY’ were mislabelled. They should be read as ‘sp-N1GDY(OH)/G’ and ‘sp-N2GDY(OH)/G’, respectively.

In Fig. 4, section (a), ‘sp-N1GDY/G (OH)’ and ‘sp-N2GDY/G (OH)’ were mislabelled. They should be read as ‘sp-N1GDY(OH)/G’ and ‘sp-N2GDY(OH)/G’, respectively. The correctly labelled Fig. 4 is given below.

In the section titled “The electronic structure of the active site relates to O₂ activation”, the O₂ dissociation barrier values for sp-N1GDY(OH)/G and Pyri-NGDY/G are given incorrectly. The correct text should be “. . . and O₂ dissociation barrier is high (1.86 eV and 1.52 eV)”.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

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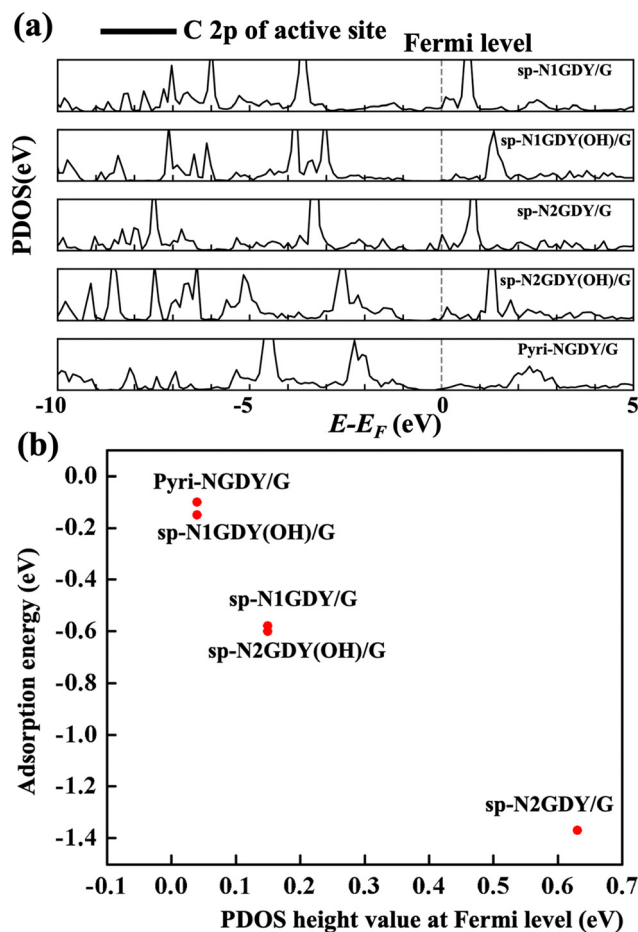


Fig. 4 (a) PDOS of C 2p of the active site in sp-N1GDY/G, sp-N1GDY(OH)/G, sp-N2GDY/G, sp-N2GDY(OH)/G, and Pyri-NGDY/G. (b) The relationship between PDOS height value at the Fermi level and the adsorption energy of O_2 .

