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CORRECTION

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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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Correction

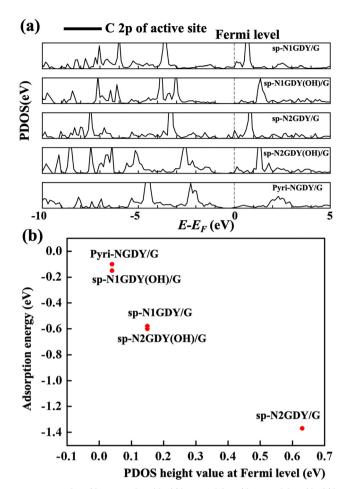


Fig. 4 (a) PDOS of C 2p of the active site in sp-N1GDY/G, sp-N1GDY(OH)/G, sp-N2GDY/G, sp-N2GDY(OH)/G, and Pyri-NGDY/G. (b) The relationship between PDOS height value at the Fermi level and the adsorption energy of O₂.