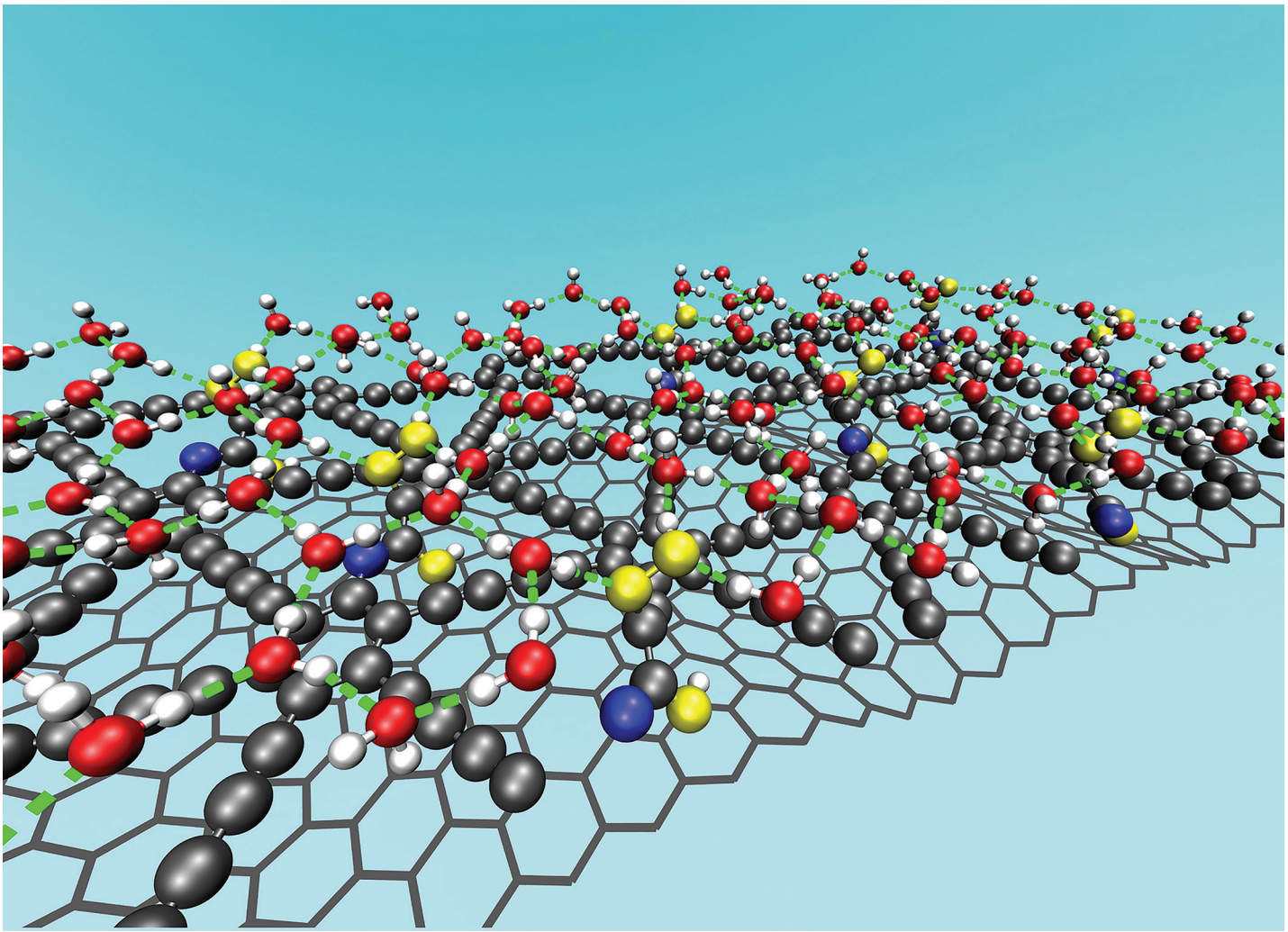
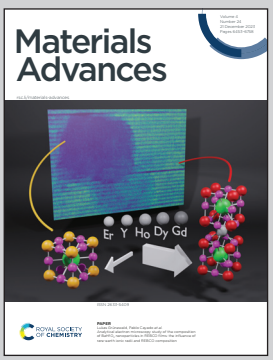


Showcasing research from Professor Morikawa's laboratory, Department of Precision Engineering, Osaka University, Osaka, Japan.

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

To reveal the active site for ORR in N-doped graphdiyne, we systematically studied the ORR mechanism on sp-N1GDY and Pyri-NGDY supported by graphene (G) using density functional theory (DFT) simulations with an explicit solvent model. OH* pre-adsorbed sp-N1GDY/G exhibits lower overpotential (0.46 V) which is close to the experiment value (0.36 V), compared with Pyri-NGDY/G (0.75 V).

As featured in:



See Yoshitada Morikawa *et al.*, *Mater. Adv.*, 2023, **4**, 6542.

ROYAL SOCIETY OF CHEMISTRY

rsc.li/materials-advances

Registered charity number: 207890