

Supporting Information

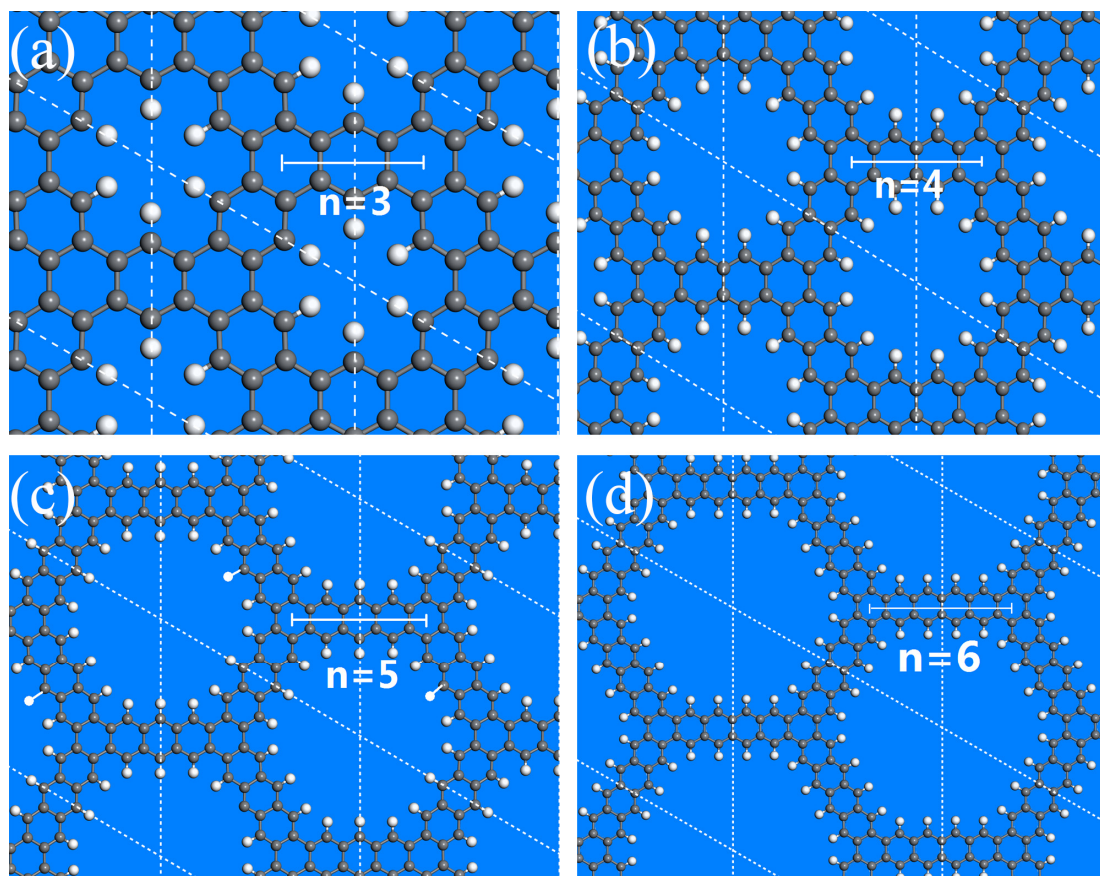


Fig. S1 The molecular structures of closed conjugated COPs (COP-Bn, $n=3,4,5,6$), (a)COP-B3, (b)COP-B4, (c)COP-B5, (d)COP-B6, the grey atoms stand for carbon atoms, and the white atoms stand for hydrogen atoms.

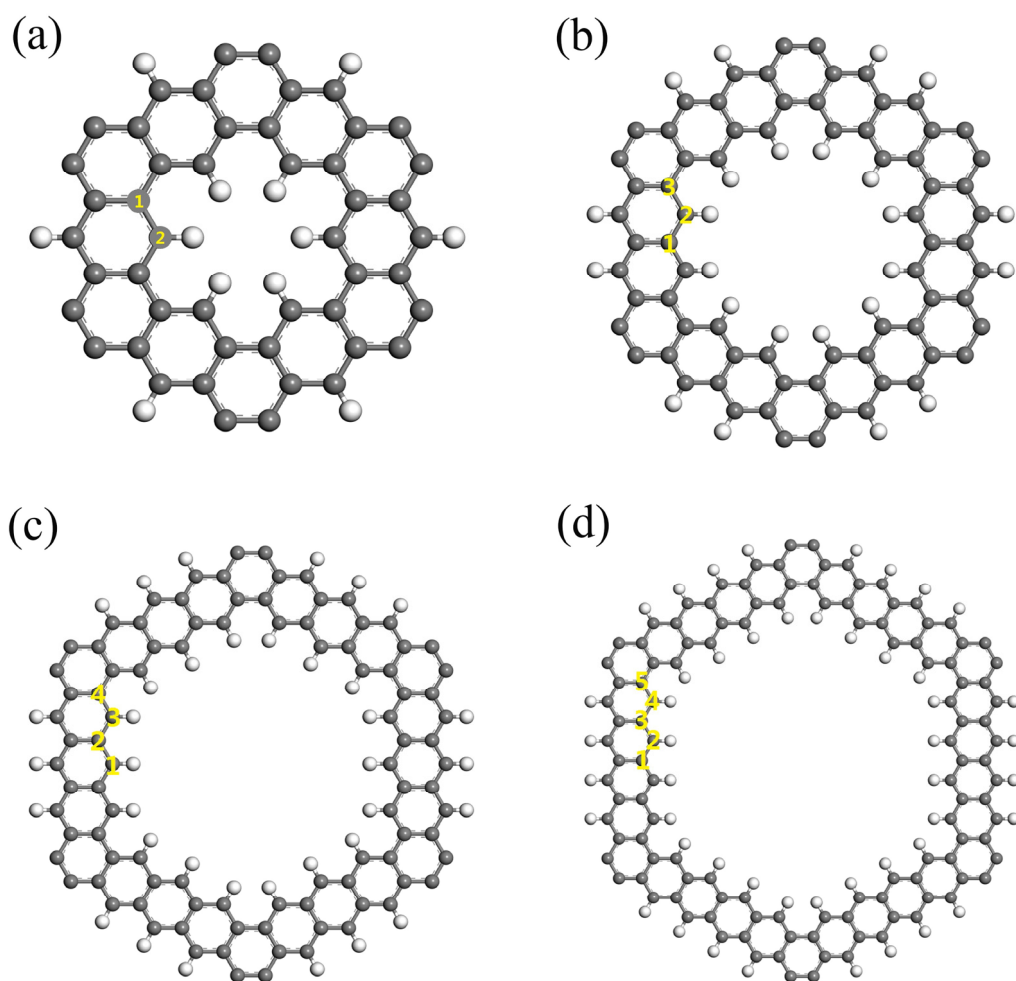


Fig. S2 The molecular structures and alternative ORR sites of closed conjugated COPs (COP-Bn, n=3,4,5,6), (a)COP-B3, (b)COP-B4, (c)COP-B5, (d)COP-B6, the grey atoms stand for carbon atoms, the white atoms stand for hydrogen atoms, and the yellow numbers stand for sites.

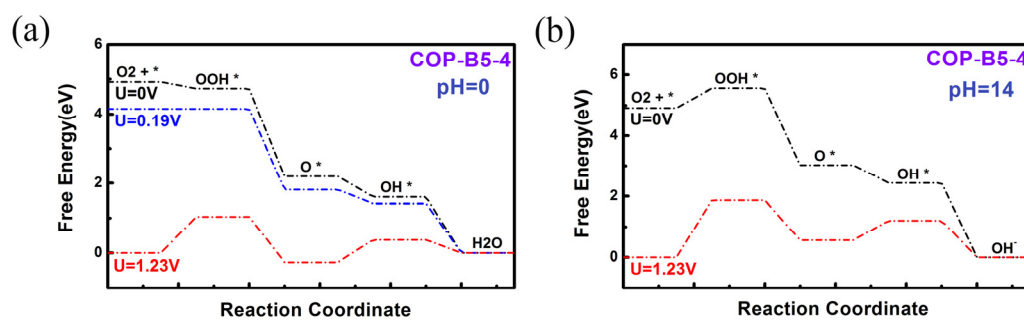


Fig. S3 Free energy curves of COP-B5 (Sites No.4, a, pH=0; b, pH=14)

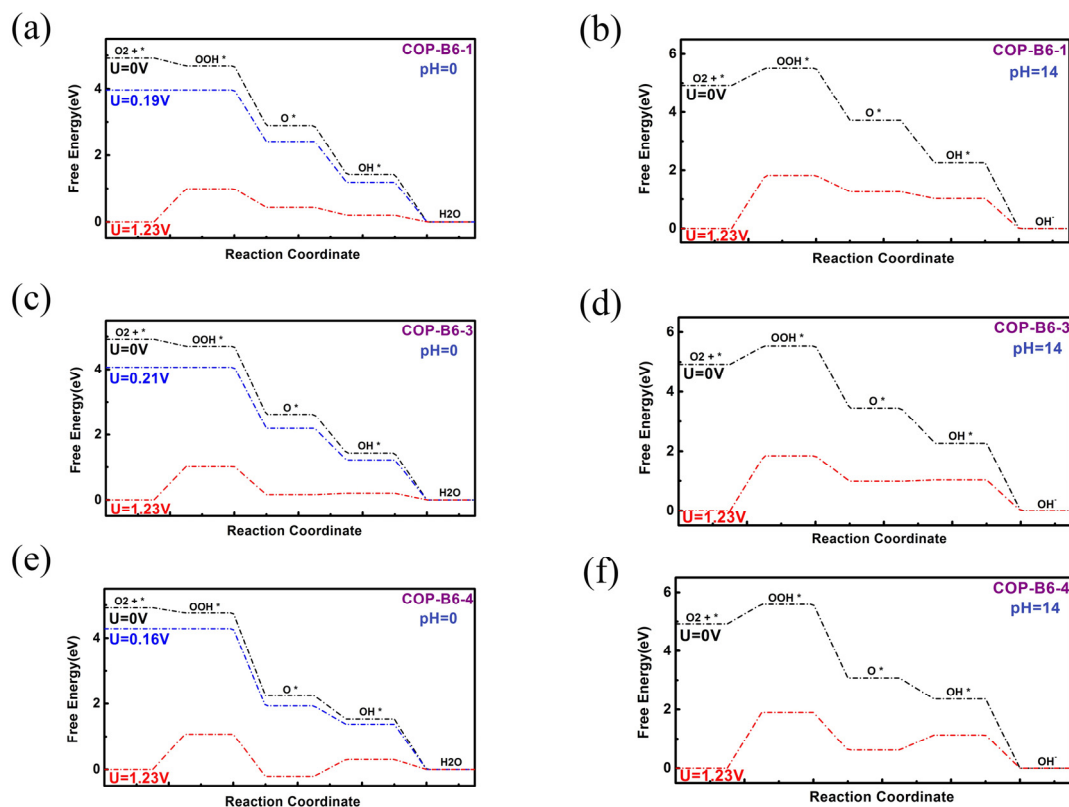


Fig. S4 Free energy curves of COP-B6 (Site No.1, a, pH=0; b, pH=14, Site No.3, c, pH=0; d, pH=14, Site No.4, e, pH=0; f, pH=14)