Supplementary Information

Understanding the High Activity of Mildly Reduced Graphene Oxide Electrocatalysts in Oxygen Reduction to Hydrogen Peroxide

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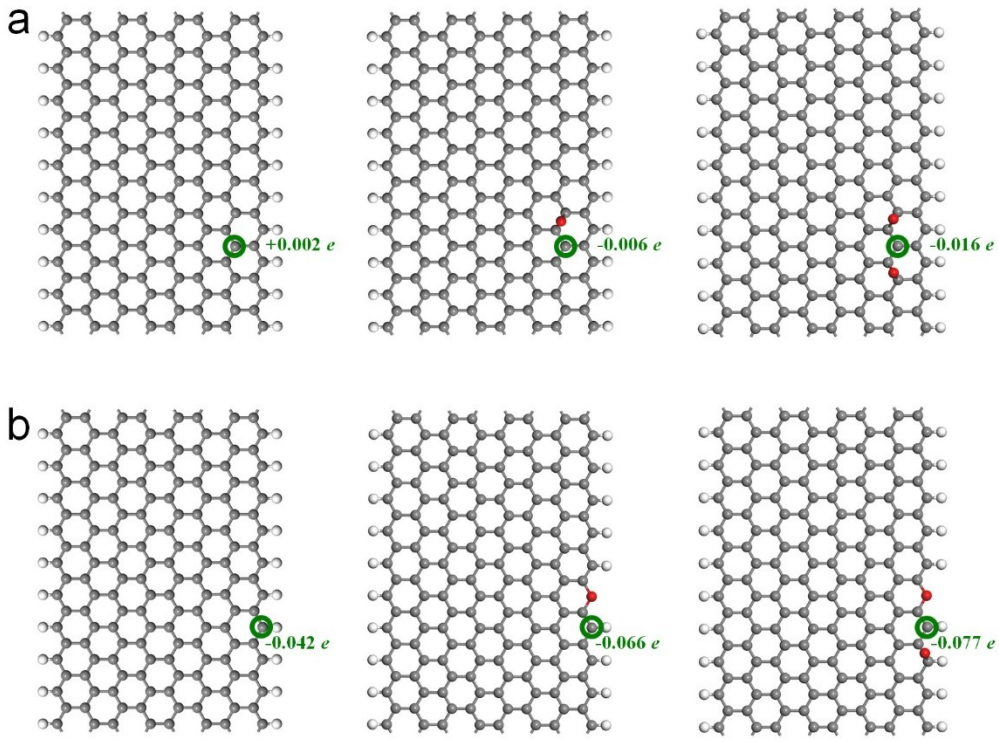

Fig. S1 The calculated charge densities of the active sites, i.e. the carbon atoms where HOO* stick to, for (a) 1EP and 2EP, and (b) 1ET and 1ET+1EP. For comparison, the calculated charge densities of carbon atoms of 8-zGNRs with no oxygen functional group (bare-G) are also shown. Here, the charge density analysis is based on the Hirshfeld method.[1] The green circles denote carbon atoms considered in the analysis, and the green numbers denote the corresponding charge densities. The calculation results show that the electrons on active sites follow the order of 2EP>1EP>bare-G and 1ET+1EP>1ET>bare-G. The grey, red and white balls represent C, O and H atoms, respectively.

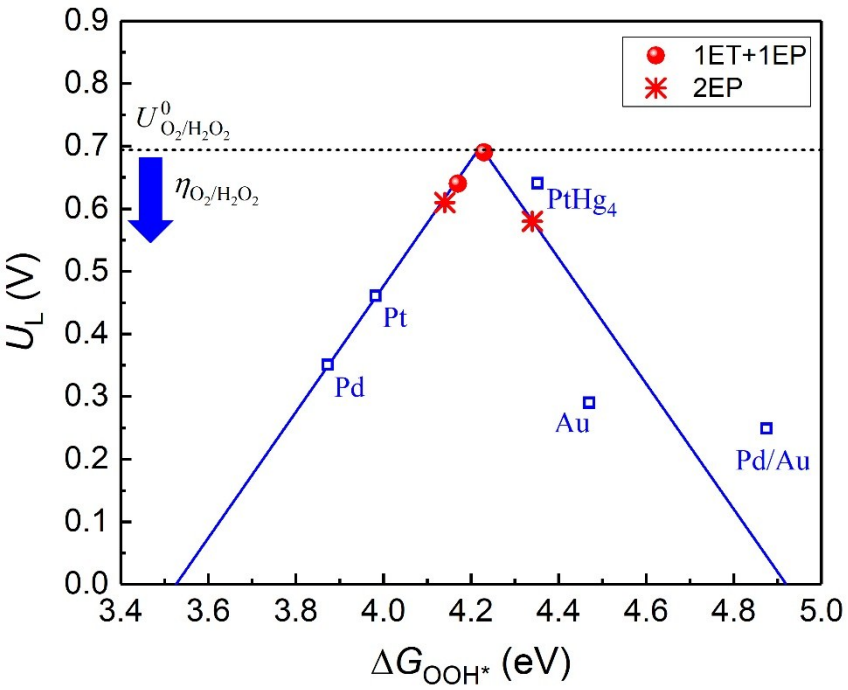

Fig. S2 The calculated U_L for H_2O_2 production of various oxygen functional group structures as a function of ΔG_{HOO^*} by using the plane-wave projector-augmented wave method as implemented in the Vienna ab initio simulation (VASP) package.[2,3] The results show that the difference of calculated values by using Dmol[3] and VASP are less than 0.06 eV.

Supplementary References

1. F. L. Hirshfeld, *Theor. Chim. Acta B*, 1977, **44**, 129.
2. G. Kresse and J. Hafner, *Phys. Rev. B*, 1994, **49**, 14251–14269.
3. G. Kresse and D. Joubert, *Phys. Rev. B*, 1999, **59**, 1758–1775.