Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Density Functional Theory Study of Oxygen Reduction Reaction Mechanism in BN co-Doped Graphene Electrocatalyst

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Supplementary Information

In alkaline medium, the complete O_2 reduction can be summarized by the reactions (1-5)[1]

$$O_2 + 2H_2O + 4e^- \rightarrow *O_2 + 2H_2O + 4e^- \quad (1)$$

$$*O_2 + 2H_2O + 4e^- \rightarrow *OOH + OH^- + H_2O + 3e^- \quad (2)$$

$$*OOH + OH^- + H_2O + 3e^- \rightarrow *O + 2(OH^-) + H_2O + 2e^- \quad (3)$$

$$*O + 2(OH^-) + H_2O + 2e^- \rightarrow *OH + 3(OH^-) + e^- \quad (4)$$

$$*OH + 3(OH^-) + e^- \rightarrow 4(OH^-) \quad (5)$$

Alternatively, OOH^- may form as a product in reaction (3) and desorb from the catalyst surface promoting $2e^-$ reduction of O_2 to peroxide.

References

1. L. Yu, X. L. Pan, X. M. Cao, P. Hu and X. H. Bao, *J. Catal.*, 2011, **282**, 183-190.