

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

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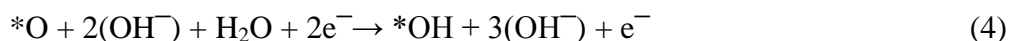
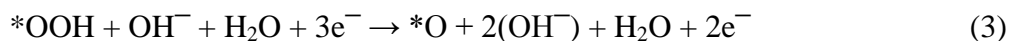
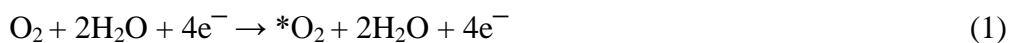
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### Supplementary Information

In alkaline medium, the complete O<sub>2</sub> reduction can be summarized by the reactions (1-5)<sup>1</sup>



Alternatively, OOH<sup>-</sup> may form as a product in reaction (3) and desorb from the catalyst surface promoting 2e<sup>-</sup> reduction of O<sub>2</sub> to peroxide.

### References

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