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

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Supplementary Information

In alkaline medium, the complete O2 reduction can be summarized by the reactions (1-5)1

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\begin{align*}
\text{O}_2 + 2\text{H}_2\text{O} + 4\text{e}^- & \rightarrow \text{O}_2 + 2\text{H}_2\text{O} + 4\text{e}^- \\
\text{*O}_2 + 2\text{H}_2\text{O} + 4\text{e}^- & \rightarrow \text{*OOH} + \text{OH}^- + \text{H}_2\text{O} + 3\text{e}^- \\
\text{*OOH} + \text{OH}^- + \text{H}_2\text{O} + 3\text{e}^- & \rightarrow \text{O} + 2(\text{OH}^-) + \text{H}_2\text{O} + 2\text{e}^- \\
\text{*O} + 2(\text{OH}^-) + \text{H}_2\text{O} + 2\text{e}^- & \rightarrow \text{*OH} + 3(\text{OH}^-) + \text{e}^- \\
\text{*OH} + 3(\text{OH}^-) + \text{e}^- & \rightarrow 4(\text{OH}^-)
\end{align*}
\]

Alternatively, OOH\(^-\) may form as a product in reaction (3) and desorb from the catalyst surface promoting 2e\(^-\) reduction of O2 to peroxide.

References