Enzyme-like Co-N-C single atom catalyst for electrocatalytic H_2O_2 production

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Hydrogen peroxide (H_2O_2) is one of the most important chemicals which plays a significant role in chemical and medical industries. The industrial production of H_2O_2 is heavily dependent on the energy-intensive anthraquinone process that requires expensive palladium catalysts. Alternatively, H_2O_2 can be produced via $2e^-$ oxygen reduction reaction (ORR) although the H_2O_2 productivity is still too low to meet the requirements for practical applications. We design and synthesize a heterogeneous Co-N-C single atom catalyst (SAC) supported on graphene that resembles the structure-dependent catalytic properties of enzymes, for highly efficient electrochemical production of H_2O_2. We demonstrate the relationship between the surrounding atomic environment of the $M-N_4$ moiety (M = transition metal) and the ORR selectivity using density functional theory (DFT) calculations and electrochemical analysis. This work demonstrates that the local atomic configuration in heterogeneous M-N-C catalysts is closely related to electrocatalytic ORR selectivity. Therefore, our result provides a new principle for designing catalysts in atomic precision for the fine-tuning of the catalytic property.