Computational design of single-atom metal-Nx/graphene catalysts for the electrochemical production of hydrogen peroxide via the oxygen reduction reaction

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Hydrogen peroxide (H_2O_2) is the simplest peroxide that is widely used as an oxidizer, bleaching agent, and antiseptic. It is produced mainly via the multi-step anthraquinone process, which requires high energy costs and massive infrastructure needs. It would be desirable if we can directly produce H_2O_2 from abundant water. Herein, we employ density functional theory (DFT) to explore the possibility of using single-atom metal-N_x/graphene catalysts to electrochemically produce H_2O_2 via the two-electron oxygen reduction reaction (ORR). We find that Co-N_4/graphene is one of the most active ORR catalysts, and slight modifications of the catalyst can lead to different selectivity. We also show, based on Bader charge analysis, that there is a correlation between the reactivity and the charge distribution of the active site, which can be used to fine-tune the catalyst.