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First-principles study of adsorption mechanisms of various sodium-oxides on N-doped graphene cathode for efficient sodium-oxygen battery

The threats posed by climate change have been reported to be driven by use of fossil fuels. Therefore, to effectively mitigate these challenges, there is need of transitioning to renewable energy sources such as solar and wind. A critical component of this transition is developing energy storage devices that not only match but exceed the energy and power densities of fossil fuels. Batteries are pivotal in this journey, as their performance is heavily influenced by the materials used in their electrodes. By tailoring and fabricating these materials, we can significantly enhance battery performance. Two dimensional materials like nitrogen-doped graphene, which offer exceptional structural and electronic properties can revolutionize these energy storage systems. In this study, density functional theory (DFT) was used to investigate the adsorption mechanisms of sodium-oxides (NaxO2, where x = 1, 2, 3, and 4) and their impact on the electronic properties of N-doped graphene cathode for efficient sodium-oxygen battery. The findings showed that various sodium-oxides, including isolated Na and O2 species, spontaneously anchor on the surface of N-doped graphene, with adsorption energies ranging from -0.31 to -0.89 eV. Additionally, the calculated charge density transfer values of 0.68, -0.33, 0.04, 0.45, 0.95, and 1.0 |e| for Na, O2, NaO2, Na2O2, Na3O2, and Na4O2 , respectively, reflect significant electronic interactions within the systems. Notably, the calculated band structures indicated enhanced metallic characteristics, suggesting that the electronic conductivity of N-doped graphene improves with the adsorption of various sodium-oxides, which is critical for electronic transport during charging processes.

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