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Probing the catalytic effects of beta-12 borophene cathode on various lithium and sodium oxide discharge products: A first-principles study

To mitigate challenges of climate change, transitioning from fossil fuels to renewable energy sources is crucial. At the center of this shift is the energy storage systems, particularly batteries with energy densities exceeding that of fossil fuels. Since an electrode of a battery determine the energy density, 2D materials like beta-12 borophene have emerged as exceptional electrode due to their excellent electronic properties. While there has been extensive research on the capabilities of beta-12 borophene as an electrode, its potential as a cathode in lithium and sodium oxygen batteries has remained unexplored, especially concerning the complete mechanisms of discharge products for lithium (LixO2) and sodium-oxides (NaxO2 , where x = 1, 2, 3, and 4). In this study, density functional theory (DFT) was used to investigate the catalytic effects of beta-12 borophene on various LixO2 and NaxO2 discharge products. The results revealed spontaneous adsorption of these products with remarkable adsorption energies ranging from -2.92 to -5.93 eV for LixO2 and -3.20 to -4.93 eV for NaxO2 systems. Additionally, low Gibbs free energy changes indicated impressive overpotentials of 3.01 V for lithium and 1.73 V for sodium systems. Our investigations also highlighted exceptionally low diffusion energy barriers between 1.05 and 0.25 eV for LixO2 and from 1.04 to 0.05 eV for NaxO2 systems. Furthermore, density of states analysis confirmed that beta-12 borophene retained its metallic characteristics, even after adsorbing insulating discharge products. The structure remained stable after heating the systems at varying temperatures of 50 to 400 K. Moreover, thermoelectric investigations revealed a slight decrease in electrical conductivity after adsorption, measuring from 1.471 × 1020 (Ω·m)−1 for the pristine material, shifting to 3.95 × 1019 (Ω·m)−1 and 1.57 × 1019 (Ω·m)−1 for Li4O2 and Na4O2 , respectively, indicating that the electrical conductivity of the material is well-maintained. Overall, our findings position beta-12 borophene as an exceptional cathode for efficient lithium and sodium oxygen batteries.

NB: This work is currently under review in the journal of energy storage

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