ABSTRACT

Sodium ion batteries (SIBs) have been attracting great interest as alternatives for grid energy storage applications in the modern world due to the sufficient natural abundance, and low cost of sodium resources. As promising cathode materials for SIBs, layered transition metal oxides exhibit high specific capacity and high energy density due to their appropriate voltage window.

In the present work, a series of binary sodium transition metals: $NaNi_{1/2}Cr_{1/2}O_2$, $NaNi_{1/2}Fe_{1/2}O_2$, $NaNi_{1/2}Co_{1/2}O_2$, and $NaNi_{1/2}Cu_{1/2}O_2$ were synthesized using sol-gel method. The synthesized samples are characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier transform infrared spectroscopy (FTIR). XRD analysis confirms that all the synthesized materials have a hexagonal structure with an R3m space group. A peak shift towards lower angle was observed for $NaNi_{1/2}Fe_{1/2}O_2$ due to increase in lattice parameters (a=b=3.07, c=15.89). SEM micrographs show hexagonal, spherical, and irregularly shaped particles. FTIR spectra indicate the presence of metal oxygen bands at 657cm-1, 650cm-1, 649cm-1, 646cm-1 for $NaNi_{1/2}Cr_{1/2}O_2$, $NaNi_{1/2}Fe_{1/2}O_2$, $NaNi_{1/2}Co_{1/2}O_2$, and $NaNi_{1/2}Cu_{1/2}O_2$. For theoretical calculations, density functional theory (DFT) was used. The structure was generated using the obtained lattice parameters from XRD. The lattice parameters obtained after optimization were in good agreement with experimental values. The investigated electronic band gap structure and density of states (DOS) reveal that all four compounds are half metallic in nature. Results reveal that the increased electronic states near the Fermi level in $NaNi_{1/2}Co_{1/2}O_2$ indicate a strong hybridization interaction between transition atoms and oxygen. Discharge voltage was calculated theoretically by computing the total energies of the optimized compounds and their de-sodianted phases. The highest discharge voltage was observed for $NaNi_{1/2}Co_{1/2}O_2$. Volume change was also calculated and found to be minimal for $NaNi_{1/2}Co_{1/2}O_2$ and $NaNi_{1/2}Cu_{1/2}O_2$ when compared to $NaNi_{1/2}Cr_{1/2}O_2$ and $NaNi_{1/2}Fe_{1/2}O_2$, implying good structural stability. Since the compound $NaNi_{1/2}Co_{1/2}O_2$ showed the highest operating potential and highest structural stability, so it is suitable as a cathode material for the fabrication of coin cell.