ABSTRACT

Lithium-ion batteries (LIBs) 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 resources. As promising cathode materials for LIBs, Ni-rich layered transition metal oxides exhibit nontoxic, high specific capacity and high energy density due to their appropriate voltage window. In the present work, a series of doped $LiNi_{1-x-y}Zn_yV_xO_2$ (x = 0.18, 0.16, and 0.14, y = 0.02, 0.04, and 0.06) were synthesized by solid-state method. The synthesized samples are characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), Energy dispersion X-ray spectroscopy (EDX) and transmission electron microscopy (TEM). XRD analysis confirms that all the synthesized materials have a hexagonal α-$NaFeO_2$ layered structure with space group R3m. The calculated parameters such as lattice values (a = b = 2.95 Å, c = 14.98 Å), unit cell volume (V=112.90 $Å^3$) and crystallite size (D = 23.11 nm) indicate the highly crystalline nature of the prepared samples. The SEM microsphere shows hexagonal, agglomerated, and irregularly shaped particles with sizes up to 0.24 μm. TEM images exhibit a grain size up to 102.5 nm with clear grain boundaries and grains were aligned in different orientations indicating polycrystalline solid. DFT-based calculations were also performed using the calculated XRD experimental data. The comprehensive investigations of structural, electronic, magnetic and electrochemical characteristics of Zn and V-doped layered $LiNiO_2$ are presented in this work. The structure of $LiNiO_2$ and doped was organized in a hexagonal arrangement inside the R3m space group The band gap was reduced due to doping indicating the metallic behavior. Electronic properties also reveal that due to the exchange coupling of orbitals, these materials exhibit a ferromagnetic nature. It is noted that through a gradual increase in the V concentration in the cathode, significant improvements were observed in the electrochemical properties of doped $LiNi_{1-x-y}Zn_yV_xO_2$. The improvements include a higher discharge capacity (48-248 mAh g^{-1}) and greater intercalation voltage (5.77–3.55 V) along with a decrease in charge transfer resistance, which led the studied compounds to a potential cathode material for lithium-ion batteries.