Supplementary

Role of electron and hole doping in NdNi_{1-x}V_xO₃ Nanostructure

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Sample S_3 and S_4 were synthesized with higher doping concentration of V. The EDX data confirms that V mostly replaces Ni ion as NdNi_{1-x}V_xO₃ (x ~0.025 for S₃ and ~0.04 for S₄).



Fig. S1 FESEM images for the pristine samples S₃, and S₄



Fig. S2 EDX spectra for the samples S₃ and S₄. Insets show the elemental composition of each sample with corresponding atomic percentages.

We have performed the X-ray photoelectron spectroscopic (XPS) technique in an ultra-high vacuum (UHV) chamber (Omicron Nanotechnology, of base pressure $\sim 1.5 \times 10^{-9}$ mbar). The UHV system was equipped with an EA125 hemispherical energy analyser along with a monochromatic X-ray light source (Al K α of photon energy 1486.6 eV). All the data were collected keeping the samples at room temperature.

The upper panel of figure S3 shows the XPS peaks correspond to Nd3d, Ni2p and O1s transitions.



Fig. S3 High resolution XPS spectra of the sample S₀, S₁, and S₂ with corresponding electronic transition of different elements.

The O1s region (figure S3a) shows peaks around 528.3 and 531 eV which can be ascribed to the sample and surface contamination, respectively [R1]. Figure S3b shows the Ni2p_{3/2} peak ~856 eV and Ni2p_{1/2} peak ~873 eV, which corresponds to trivalent Ni [R2]. We also observed characteristic satellites at about 862 and 880 eV. The Nd3d level spectra (figure S3c) shows peaks ~882 and 1004 eV correspond to Nd3d_{5/2} and Nd3d_{3/2} transitions, respectively. We were also able to observe the low binding energy satellites, which is the characteristic feature of Nd multiplet [R3]. For all the three samples we observe similar spectra for Nd, Ni, and O. However, the position of V lines varies for samples S₁, and S₂. The lower panel of figure S3 displays the existence of V and its corresponding valence state. Sample S₁ and S₂ confirms the presence of Vanadium, whereas for sample S₀, no trace of V is observed (figure S3d). The V 2p_{3/2} peak is observed ~ 513.4 eV for sample S₁, whereas the same is observed ~ 516.2 eV for sample S₂ (figure S3e-f). The position of V 2p_{3/2} peak confirms that V is in +2 state [R4] in sample S₁, where as it is in +4 state [R5] in sample S₂, as also argued from resistivity, Raman spectroscopic and XRD analysis.



Fig. S4 Rietveld refined X-ray diffraction pattern of samples (a) S₃, (b) S₄. Impurity peaks are marked by '*' sign.



Fig. S5 Schematic structure of NdNi_{1-x}V_xO₃ unit cell of sample (a) S₀ (x=0.0), (b) S₁ (x=0.1), and (c) S₂ (x=0.2), drawn using VESTA software.



Fig. S6 Raman spectra as a function of temperature for NdNi_{1-x}V_xO₃ (x = 0.01) nanostructure (sample S₁)



Figure S7. Resistivity plots as a function of temperature for NdNi_{1-x}V_xO₃ (x = 0.01) nanostructure for both heating and cooling cycle with a hysteresis ~ 10 K.

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