Supplementary information to Structural and Electrical Properties of Lithium Substituted Niobo Vanadate Glasses Doped with Nickel Ferrite

This supplementary information contains the details of basic characterization of VNL glasses and Nickel Ferrite as well as tables of various parameters used to fit the Cole-Cole representation of impedance data.

S1. Physical property measurements and characterization:

Density of the prepared glasses were determined using the Archimedes principle, to an accuracy of ±0.004 g/cc. Xylene was used as an immersion liquid with a density of 0.864 g/cc (declared by the manufacturer). A high resolution electronic weighing balance (with an accuracy of 0.0001 g) was used to measure the weights of the samples in air and liquid. The molar volume was calculated using the equation $V_m = \frac{M}{\rho}$, where M is the molecular weight of the glass sample, which was calculated as $M = \sum x_i w_i$, where x_i and w_i are the mole fraction and molecular weight of the component i and ρ is the density, respectively. The values are listed in Table 1 in the main manuscript.

The concentration of alkali ions in the general formula $x\%A_bB_c$: ($x\%Li_2O$) can be calculated from $n(A) = \frac{b\ x\ N}{100\ V_m}$, where, x, N *and* V_m are mole percentage, Avogadro number and molar volume, respectively. The separation between like ions was calculated using the formula $r = (1/n)^{1/3}$. The distance between Li and O was calculated by assuming that O lies at half distance between two Li atoms.

S2 EPR of VNL glasses:

The oxidation state of vanadium in the glass was confirmed by EPR measurement of the glass. The absence of vanadium hyperfine signature confirms that the vanadium is in V^{5+} state i.e., it forms a VO_5 structure. Fig.**S1** shows the EPR spectra of un-doped and Nickel Ferrite doped glasses. The central broad absorption is because of the cavity resonance. The central absorption at around 3360.20 G and 3350.15 G. for VNL 15 and VNLFe 15, respectively. The sharp absorption at around 3491.09 and 1723.07 G for VNL is the signature of DPPH which is used as reference.

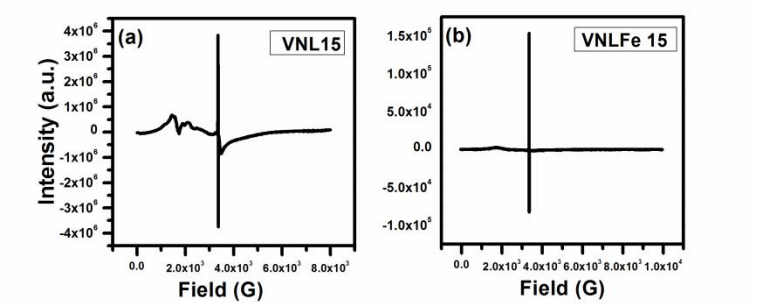

Fig. **S1** (a) and (b) EPR of VNL 15 and VNLFe 15 (VNL 15 doped with Nickel Ferrite.)

S3 Characterization of Nickel Ferrite:

S3.1 XRD of Nickel Ferrite (NF)

The XRD of NF ($NiFe_2O_4$) is shown in Fig.**S2**. The crystal structure and particle size of nano particles have been investigated using Scherer's relation using equation $D = \frac{K\lambda}{\beta \cos\theta}$

where λ is the wavelength of X-ray diffraction (1.5406 Å), K is a constant taken as 0.89, θ is the diffraction angle and β is the full width half maximum (FWHM) [S1]. The crystallite size was calculated and the average crystallite size was found to be 51nm.

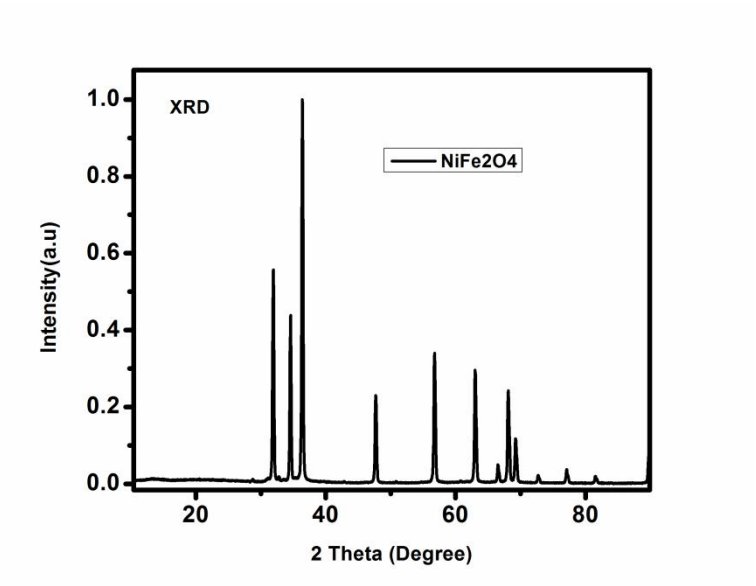

Fig. S2: XRD of Nickel Ferrite

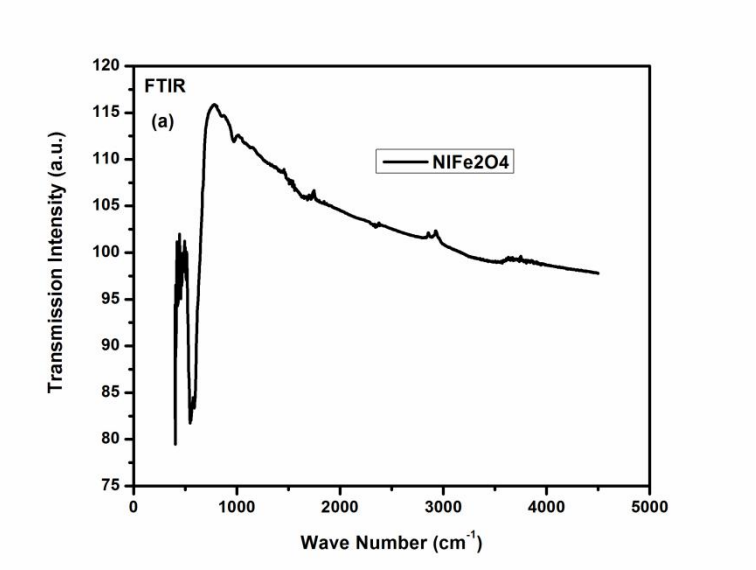

Fig. S3: FTIR of Nickel Ferrite

S3.2 SEM of Nickel Ferrite (NF)

Microstructural information of $NiFe_2O_4$ (NF) was obtained using scanning electron microscopy (SEM). Field emission scanning electron microscopy was used at different magnifications to obtain a representative crystallite size and separation distance between pores in the synthesized nickel ferrite. The sample was examined at an accelerating voltage of 5 kV. The entire set-up was interfaced with a computer which enabled the direct recording of micrographs. The SEM information of nickel ferrite ($NiFe_2O_4$) is shown in Fig.6. As can be seen from Fig.6 the sample is uniform, almost spherical structural morphology with narrow size distribution but with agglomeration to some extent.

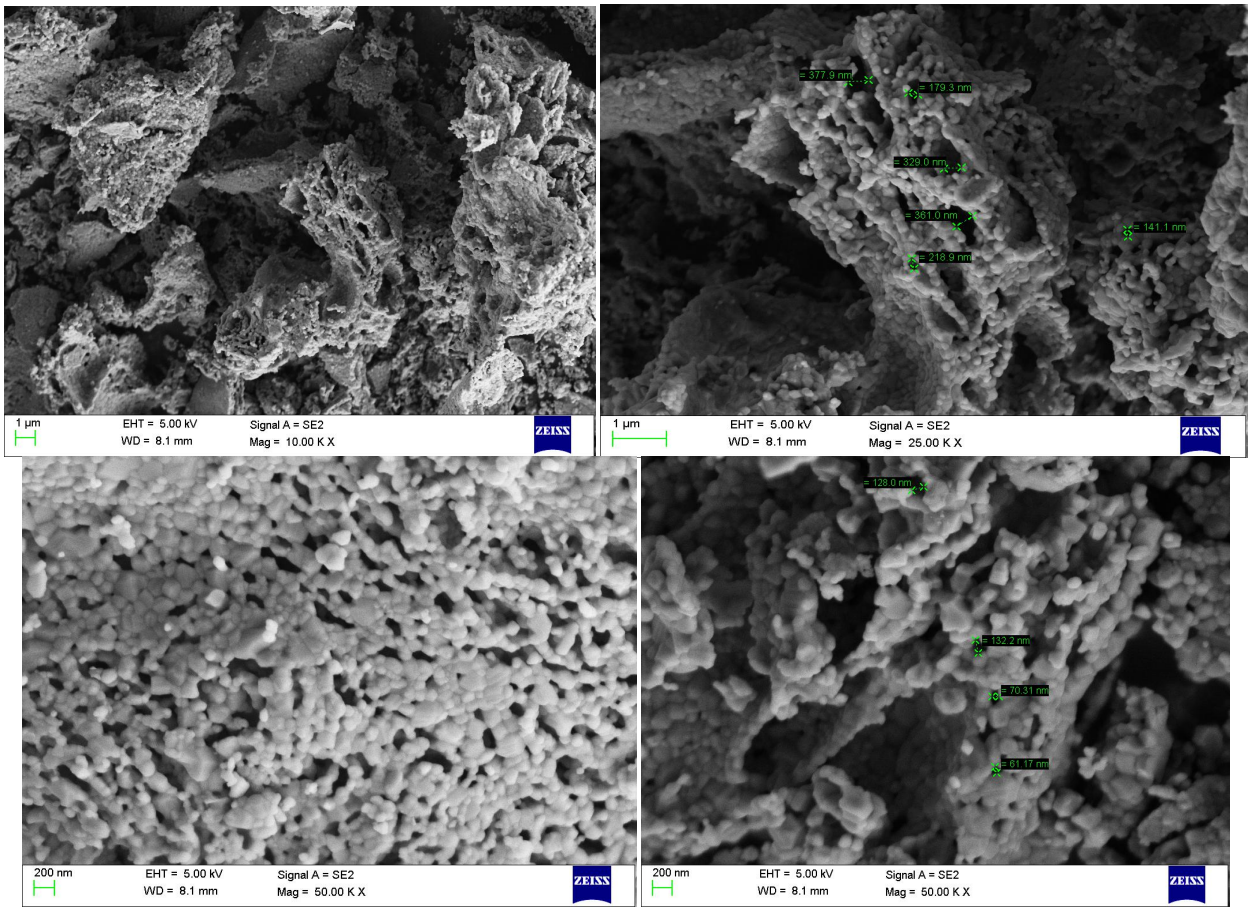

Fig. S4 : SEM Images of Nickel Ferrite ($NiFe_2O_4$)

S4 Tables and values of various parameters used in fitting the equivalent circuit elements to Cole-Cole plots. The meaning of the symbols and the significance are discussed in the main text.

Table S1: (a) Parameters used to fit measured Cole-Cole plot of **VNL 15** using two RC circuits (R_s+C_1/R_1+C_2/R_2) :Inadequate fitting

Temperature (°C) VNL 15	$R_s(\Omega)$	C_1(F)	$R_1(k\Omega)$	C_2(F)	$R_2(k\Omega)$
120	602.8	4.481×10^{-12}	89. 18	1.076×10^{-9}	52. 89
140	506.4	4.82×10^{-12}	46. 22	1.191×10^{-9}	34. 63
160	456.6	1.172×10^{-9}	22. 43	4.698×10^{-12}	24. 70
180	467.3	1.137×10^{-9}	13. 17	5.091×10^{-12}	13. 61
200	425.9	5.679×10^{-12}	7. 33	1.02×10^{-9}	5. 99
220	393.5	1.055×10^{-9}	2. 76	6.58×10^{-12}	3. 86

Table S1: (b) Parameters used to fit measured Cole-Cole plot of **VNL 15** using two RQ circuits (R_s+C_1/R_1+C_2/R_2): Adequate fitting

Temperature (°C)	$R_S(\Omega)$	ϕ_1	$Q_1\left(Fs^{\phi_1-1}\right)$	$R_1(k\Omega)$	ϕ_2	$Q_2\left(Fs^{\phi_2-1}\right)$	$R_2(k\Omega)$

VNL 15							
120	4.6×10^{-24}	0.915	16.98×10^{-12}	94.75	0.933	2.761×10^{-9}	48.06
140	-133.5	0.904	21.87×10^{-12}	48.75	0.927	3.021×10^{-9}	33.38
160	4.39	0.903	23.68×10^{-12}	26.28	0.930	2.826×10^{-9}	22.15
180	-84.86	0.884	34.84×10^{-12}	14 94	0.963	2.011×10^{-9}	13.13
200	1.79×10^{-12}	0.886	37.65×10^{-12}	8.08	0.927	2.871×10^{-9}	6.18
220	1.55	0.875	50.08×10^{-12}	4.40	0.934	2.826×10^{-9}	2.66

Table S2: (a) Parameters used to fit measured Cole-Cole plot of **VNL 20** using two RC circuits (R_s+C_1/R_1+C_2/R_2): Inadequate fitting

Temperature (°C) VNL 20	$R_s(\Omega)$	C_1(F)	$R_1(k\Omega)$	C_2(F)	$R_2(k\Omega)$
120	40.46	3.05×10^{-9}	4.773×10^{3}	5.61×10^{-12}	410.75
140	239	3.17×10^{-9}	3.511×10^{3}	6.13×10^{-12}	96.71
160	8.41	6.16×10^{-12}	140.83	1.32×10^{-9}	261.94
180	47.6	2.17×10^{-9}	1.267×10^{3}	6.42×10^{-12}	77.44
200	1 552	1.62×10^{-9}	280. 57	8.04×10^{-12}	39.15
220	421.5	1.56×10^{-9}	240. 80	7.44×10^{-12}	21.50

Table S2: (b) Parameters used to fit measured Cole-Cole plot of **VNL 20** using two RQ circuits (R_s+C_1/R_1+C_2/R_2): Adequate fitting

Temperature (°C) VNL 20	$R_S(\Omega)$	ϕ_1	$Q_1\left(Fs^{\phi_1-1}\right)$	$R_1(k\Omega)$	ϕ_2	$Q_2\left(Fs^{\phi_2-1}\right)$	$R_2(k\Omega)$
120	170.5	0.955	2.20×10^{-9}	620.48	0.955	11.27×10^{-12}	406.74
140	4.80	0.989	1.80×10^{-9}	497.79	0.863	55.39×10^{-12}	102.34

160	-421.8	0.940	2.69×10^{-9}	793.21	0.882	40.37×10^{-12}	160.31
180	0.58	0.821	5.46×10^{-9}	743.24	0.911	26.88×10^{-12}	77.16
200	3.88	0.906	4.03×10^{-0}	670.61	0.862	67.22×10^{-12}	43.04
220	200.7	0.872	5.24×10^{-9}	703.65	0.921	27.55×10^{-12}	21.90

Table S3: (a) Parameters used to fit measured Cole-Cole plot of **VNL 25** using two RC circuits (R_s+C_1/R_1+C_2/R_2): Inadequate fitting

Temperature (°C) **VNL 25**	**R_s(Ω)**	**C_1(F)**	**R_1(kΩ)**	**C_2(F)**	**R_2(kΩ)**
120	134.2	5.17×10^{-12}	389. 33	12×10^{-12}	20.54
140	291.4	0.14×10^{-9}	2.02×10^{3}	4.40×10^{-12}	287.08
160	313.8	4.70×10^{-12}	146.64	0.97×10^{-9}	435.88
180	29.7	4.78×10^{-12}	104.24	1.16×10^{-9}	417.92
200	1627	1.04×10^{-9}	318.36	5.93×10^{-12}	46.09
220	1947	1.04×10^{-9}	166.80	6.90×10^{-12}	29.48

Table S3: (b) Parameters used to fit measured Cole-Cole plot of **VNL 25** using two RQ circuits (R_s+C_1/R_1+C_2/R_2): Adequate fitting

Temperature (°C) **VNL 25**	**R_S(Ω)**	ϕ_1	$Q_1\left(Fs^{\phi_1-1}\right)$	**R_1(kΩ)**	ϕ_2	$Q_2\left(Fs^{\phi_2-1}\right)$	**R_2(kΩ)**
120	13.84	0.996	17.06×10^{-12}	607.49	0.857	15.36×10^{-12}	290.55

140	2.14	0.968	0.72 x10^{-9}	396.79	0.876	31.6x10^{-12}	360.09
160	1.59	0.831	4.21 x10^{-9}	829.46	0.898	24.42x10^{-12}	155.61
180	155.4	0.963	1.57x10^{-9}	494.26	0.905	22.6x10^{-12}	113 28
200	95.84	0.926	2.12 x10^{-9}	417.06	0.857	56.04x10^{-12}	50.75
220	0.71x10^{-6}	0.789	8.72x10^{-9}	678.88	0.865	52.65x10^{-12}	30.80

Table S4: (a) Parameters used to fit measured Cole-Cole plot of **VNLFe 15** using two RC circuits (R_s+C_1/R_1+C_2/R_2): Inadequate fitting

Temperature (°C) **VNLFe 25**	**R_s(Ω)**	**C_1(F)**	**R_1(k Ω)**	**C_2(F)**	**R_2(k Ω)**
120	3157	18.91x10^{-12}	47.95	2.02x10^{-9}	213.30
140	497.6	2.18x10^{-9}	313.27	13.91 x10^{-12}	25. 54
160	470	14.56 x10^{-12}	14.18	2.12 x10^{-9}	220.12
180	647.2	2.05x10^{-9}	136.94	17.38 x10^{-12}	7.80
200	277.8	2.06x10^{-9}	162.39	19.76 x10^{-12}	5 14
220	349.7	18.33x10^{-9}	2.62	2.23x10^{-9}	65.12
240	307.3	20.88e-12	1 445	2.82e-9	8 959

Table S4: (b) Parameters used to fit measured Cole-Cole plot of **VNLFe 15** using two RQ circuits (R_s+C_1/R_1+C_2/R_2): Adequate fitting

Temperature (°C) **VNLFe 15**	**R_S(Ω)**	ϕ_1	$Q_1\left(Fs^{\phi_1-1}\right)$	**R_1(k Ω)**	ϕ_2	$Q_2\left(Fs^{\phi_2-1}\right)$	**R_2(k Ω)**
120	26.31	0.874	6.56x10^{-9}	406.12	0.810	0.27x10^{-9}	54.70

140	23.01	0.888	6.20×10^{-9}	924.94	0.809	0.30×10^{-9}	29.41
160	100.5	0.872	7.14×10^{-9}	683.73	0.826	0.25×10^{-9}	15.57
180	744.9	0.902	5.26×10^{-9}	209. 90	0.991	21.26×10^{-12}	7.43
200	370.6	0.910	4.99×10^{-9}	213.65	0.930	55.4×10^{-12}	4.53
220	60.14	0.956	3.61×10^{-9}	68.46	0.775	0.74×10^{-9}	3.14
240	9.72×10^{-12}	0.919	7.31×10^{-9}	9.92	0.767	0.84×10^{-9}	1.82

Table S5: (a) Parameters used to fit measured Cole-Cole plot of **VNLFe 20** using two RC circuits (R_s+C_1/R_1+C_2/R_2): Inadequate fitting

Temperature (°C) **VNLFe 20**	**$R_s(\Omega)$**	**C_1(F)**	**$R_1(k\Omega)$**	**C_2(F)**	**$R_2(k\Omega)$**
120	107.8	9.98×10^{-12}	59.0	5.67×10^{-12}	900.15
140	390.6	1.36×10^{-9}	1.44×10^{3}	4.26×10^{-12}	465.53
160	145.2	1.07×10^{-9}	1.86×10^{3}	4.62×10^{-12}	231.20
180	161	1.05×10^{-9}	280. 81	4.55×10^{-12}	109.94
200	1 180	1.19×10^{-9}	297. 87	5.18×10^{-12}	57.63
220	588.2	1.18×10^{-9}	194. 94	5.21×10^{-12}	31.36
240	541.7	5.59×10^{-12}	17.32	1.43×10^{-9}	90.94

Table S5: (b) Parameters used to fit measured Cole-Cole plot of **VNLFe 20** using two RQ circuits (R_s+C_1/R_1+C_2/R_2): Adequate fitting

Temperature (°C) **VNLFe 20**	**$R_S(\Omega)$**	ϕ_1	$Q_1\left(Fs^{\phi_1-1}\right)$	**$R_1(k\Omega)$**	ϕ_2	$Q_2\left(Fs^{\phi_2-1}\right)$	**$R_2(k\Omega)$**

120	8.97	0.970	$8.10x10^{-12}$	927.07	0.997	$14.52x10^{-12}$	53.25
140	32.4	0.805	$4.12x10^{-9}$	572.44	0.911	$17.33x10^{-12}$	451.06
160	168.1	0.968	$1.48x10^{-12}$	829.55	0.942	$11.44x10^{-12}$	238.23
180	286.4	0.967	$1.63x10^{-9}$	934.64	0.955	$9.42x10^{-12}$	117.28
200	107	0.956	$1.84x10^{-9}$	538.87	0.905	$23.04x10^{-12}$	61.93
220	-510	0.947	$2.08x10^{-9}$	329.24	0.841	$68.61x10^{-12}$	35.41
240	556.3	0.923	$3.17x10^{-9}$	137.16	0.989	$6.81x10^{-12}$	17.18

Table S6: (a) Parameters used to fit measured Cole-Cole plot of **VNLFe 25** using two RC circuits (R_s+C_1/R_1+C_2/R_2): Inadequate fitting

Temperature (°C) **VNLFe 25**	**R_s(Ω)**	**C_1(F)**	**R_1(kΩ)**	**C_2(F)**	**R_2(kΩ)**
120	566.9	$30.69x10^{-12}$	55. 94	$1.31x10^{-9}$	598.90
140	175.1	$3.81x10^{-9}$	890.23	$5.03x10^{-12}$	295.01
160	378.4	$5.11x10^{-12}$	135. 03	$1.46x10^{-9}$	103.99
180	538.5	$2.30x10^{-9}$	130.35	$5.40x10^{-12}$	69.35
200	415	$1.01x10^{-9}$	$1.25x10^{6}$	$5.57x10^{-12}$	33.33
220	569.7	$1.05x10^{-9}$	490.88	$6.26x10^{-12}$	16.29
240	572.9	$7.62x10^{-12}$	7.60	$1.16x10^{-9}$	73.57

Table S6: (b) Parameters used to fit measured Cole-Cole plot of **VNLFe 25** using two RQ circuits (R_s+C_1/R_1+C_2/R_2): Adequate fitting

Temperature (°C) VNLFe 25	$R_S(\Omega)$	ϕ_1	$Q_1\left(Fs^{\phi_1-1}\right)$	$R_1(k\Omega)$	ϕ_2	$Q_2\left(Fs^{\phi_2-1}\right)$	$R_2(k\Omega)$
120	168.3	0.920	4.10×10^{-9}	526.23	0.787	0.72×10^{-9}	74.69
140	3.15	0.754	36.16×10^{-9}	787.18	0.888	28.96×10^{-9}	317. 01
160	0.04	0.930	4.27×10^{-9}	245.73	0.886	32.15×10^{-12}	154.74
180	-287.8	0.705	41.75×10^{-9}	636.79	0.883	35.75×10^{-12}	72.99
200	173.1	0.999	0.93×10^{-9}	702. 22	0.893	33.12×10^{-12}	35.94
220	4.85	0.937	1.93×10^{-9}	749. 53	0.856	68.68×10^{-12}	17.79
240	440.8	0.907	3.15×10^{-9}	112. 85	0.967	13.06×10^{-12}	7.56

The range of the variation of these values are summarized and presented in main text as **Table 2**.