Supplementary Information

Study on the decisive factor for metal-insulator transition in LaVO$_3$ Mott-Hubbard insulator

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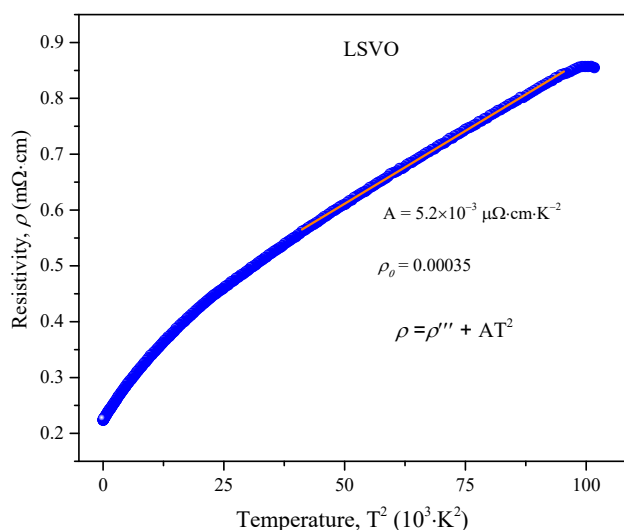*kimoon.lee@kunsan.ac.kr (Kimoon Lee)*

Fig. S1. Unsatisfactory fit of resistivity using Fermi-liquid-like behavior for LSVO.

Table SI. *The goodness of fitting, selected bond lengths, orthorhombic lattice strain, tolerance factor, and octahedral distortion parameters obtained from structural refinement of XRD data of LVO, LCVO, and LSVO.*

Sample	LVO	LCVO	LSVO
c/a ratio	1.413	1.412	1.410
GOF	10.7	11.8	17.4
<V–O1> (Å)	1.999(3)	1.964(1)	1.965(2)
<V–O2> (Å)	2.018 (9)	1.973 (1)	1.987(1)
<V–O2> (Å)	1.983 (9)	1.970 (1)	1.972(1)
<V–O> (Å)	2.000 (1)	1.969 (1)	1.974 (1)
Orthorhombic lattice strain	0.00027	-0.0010	-0.0060
Octahedral distortion $10^{-7}\Delta_d$	0.83	0.86	3.4
Tolerance factor	0.911	0.908	0.920

Table SII. *Peak parameters obtained from the deconvolution of V 2p together with O 1s spectra for LVO, LCVO, and LSVO.*

Samples		LVO		LCVO		LSVO	
Peak parameters / Peak types		FWHM (eV)	Position (eV)	FWHM (eV)	Position (eV)	FWHM (eV)	Position (eV)
$2p_{3/2}$	V^{3+}	2.3	516.1	1.9	515.9	2.0	515.8
	V^{4+}	1.3	517.0	1.3	517.1	1.3	517.1
$2p_{1/2}$	V^{3+}	3.0	523.5	3.0	523.3	3.0	523.1
	V^{4+}	2.9	524.4	2.8	524.5	2.9	524.4
O 1s	1st peak	1.4	529.8	1.5	529.9	1.5	529.8
	2nd peak	2.5	531.6	2.3	531.5	2.7	531.7
Ratio V^{4+}/V^{3+}		1.1		1.6		1.9	

Table SIII. *Room temperature conductivity, Seebeck coefficient, carrier concentration and mobility.*

Sample	σ (S/cm)	S (μV/K)	*PF (mW/mK²)*	p (10^{22} cm^{-3})	μ (cm²/Vs)
LVO	0.09	441.5	1.87		
LCVO	804.5	2.5	0.51	1.13	0.443
LSVO	908.9	0.47	0.10	1.12	0.517

Table SIV. *Electrical parameters obtained from modeling resistivity data using equations (5-9)*

Sample	E_a (eV)	ρ' (Ω·cm)	ρ'' (Ω·cm)	T_0 (K)	$N(E_F)$ (eV^{-1}·cm^{-3})	ρ''' (Ω·cm)	A (μΩ·cm·K²)
LVO	0.16	1.7	2×10^{-15}	4.7×10^8	2.4×10^{19}		
LCVO						0.00084	$(1.5/1.1) \times 10^{-2}$
LSVO						0.00022	1.2×10^{-1}