Supplementary Material (ESI) for Dalton Transactions

Syntheses, Crystal Structures, and Properties of Three New Lanthanum(III) Vanadium Iodates

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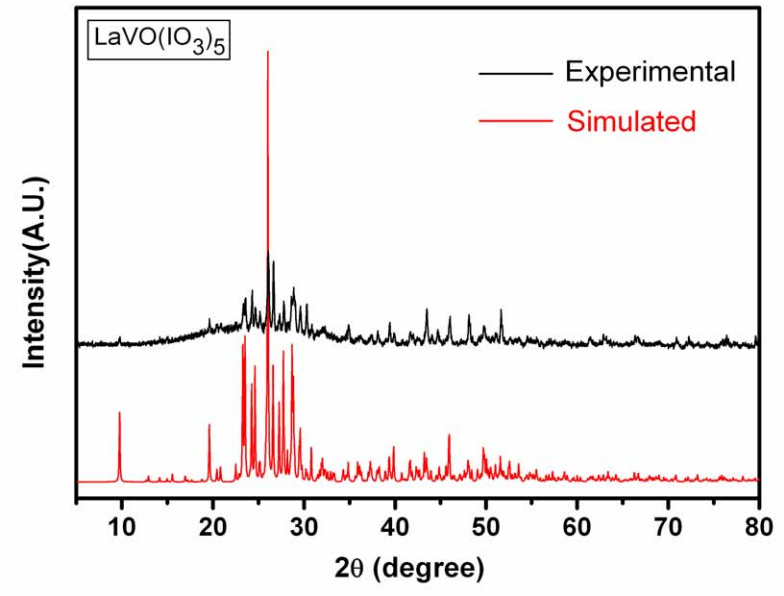
Supporting Information

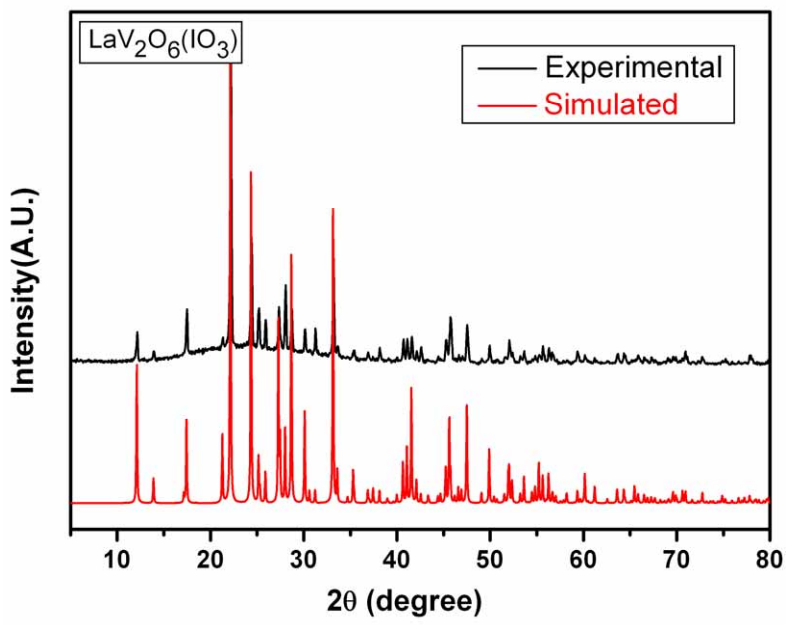
Table S1. The state energies (eV) of the lowest conduction band (L-CB) and the highest valence band (H-VB) of the three compounds.

Compound	k-point	L-CB	H-VB
$LaVO(IO_3)_5$	Z (0.000, 0.000, 0.500)	1.80538	-0.03615
	G (0.000, 0.000, 0.000)	1.77737	-0.02481
	Y (0.000, 0.500, 0.000)	1.80275	-0.03083
	A (-0.500, 0.500, 0.000)	1.70472	-0.03289
	B (-0.500, 0.000, 0.000)	1.70165	-0.02831
	D (-0.500, 0.000, 0.500)	1.73478	0
	E (-0.500, 0.500, 0.500)	1.73592	-9.60018E-4
	C (0.000, 0.500, 0.500)	1.80838	-0.04235
	G (0.000, 0.000, 0.000)	2.56173	0
	Z (0.000, 0.000, 0.500)	2.55052	-0.11088
	T (-0.500, 0.000, 0.500)	2.57004	-0.13066
	Y (-0.500, 0.000, 0.000)	2.65569	-0.0932

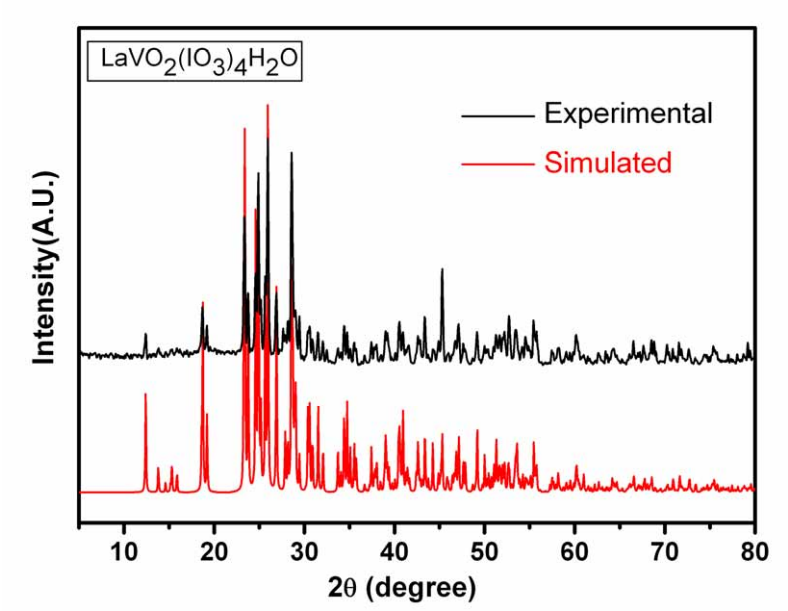
$LaV_2O_6(IO_3)$	S (-0.500, 0.500, 0.000)	2.70836	-0.13874
	X (0.000, 0.500, 0.000)	2.64429	-0.10728
	U (0.000, 0.500, 0.500)	2.55247	-0.15366
	R (-0.500, 0.500, 0.500)	2.58301	-0.1765
$LaVO_2(IO_3)_4 \cdot H_2O$	Z (0.000, 0.000, 0.500)	2.86923	-0.068798
	G (0.000, 0.000, 0.000)	2.77154	-0.09801
	Y (0.000, 0.500, 0.000)	2.88285	-0.10217
	A (-0.500, 0.500, 0.000)	2.84439	-0.06138
	B (-0.500, 0.000, 0.000)	2.70804	-0.06181
	D (-0.500, 0.000, 0.500)	2.66687	0
	E (-0.500, 0.500, 0.500)	2.7497	-0.00754
	C (0.000, 0.500, 0.500)	2.92196	-0.08085



(a)

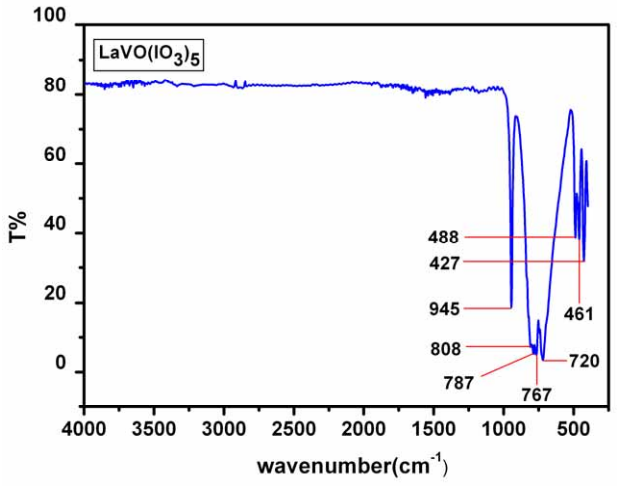


(b)

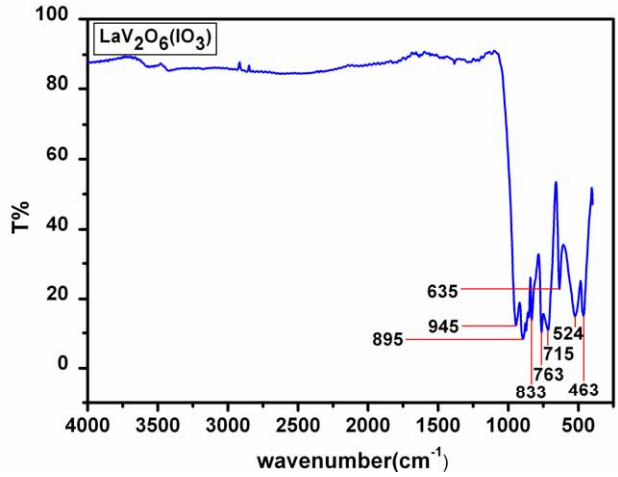


(c)

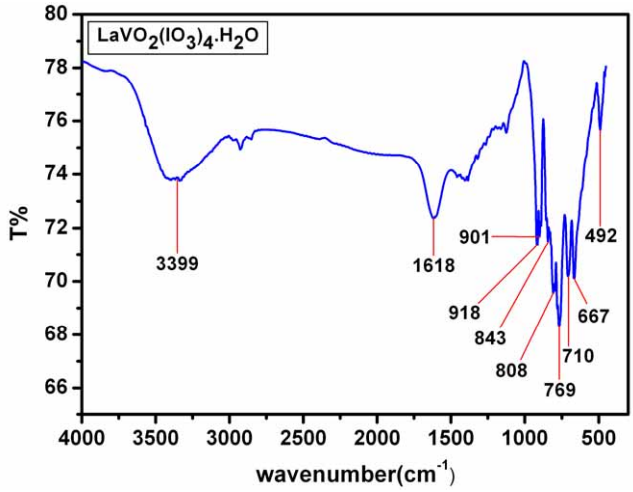
Figure S1. Experimental and simulated X-ray powder diffraction patterns for $LaVO(IO_3)_5$ (a), $LaV_2O_6(IO_3)$ (b), and $LaVO_2(IO_3)_4 \cdot H_2O$ (c).



(a)



(b)



(c)

Figure S2. The infrared spectra for $LaVO(IO_3)_5$ (a), $LaV_2O_6(IO_3)$ (b), and $LaVO_2(IO_3)_4{\cdot}H_2O$ (c).

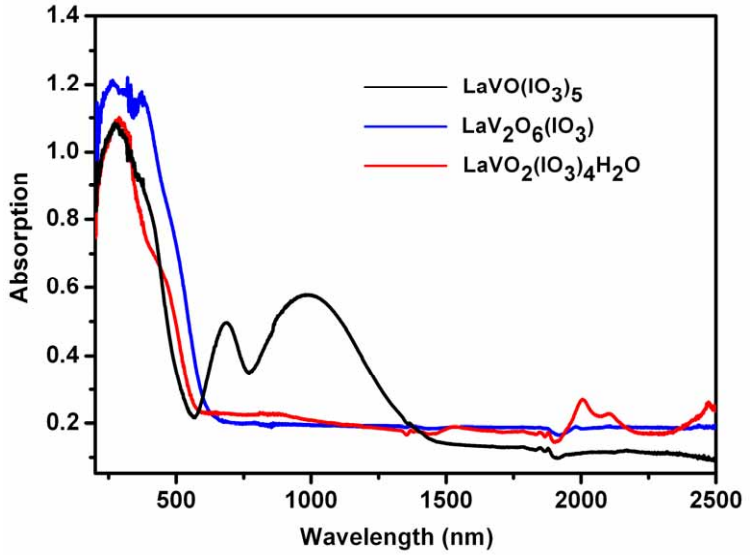


Figure S3. UV absorption spectra for $LaVO(IO_3)_5$, $LaV_2O_6(IO_3)$, and $LaVO_2(IO_3)_4{\cdot}H_2O$.

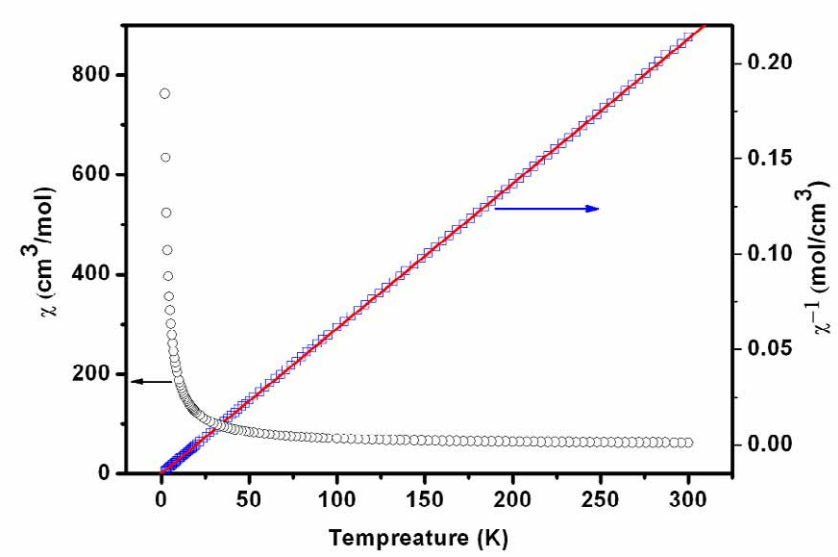


Figure S4. χ versus T and 1/χ versus T plots for $LaVO(IO_3)_5$.

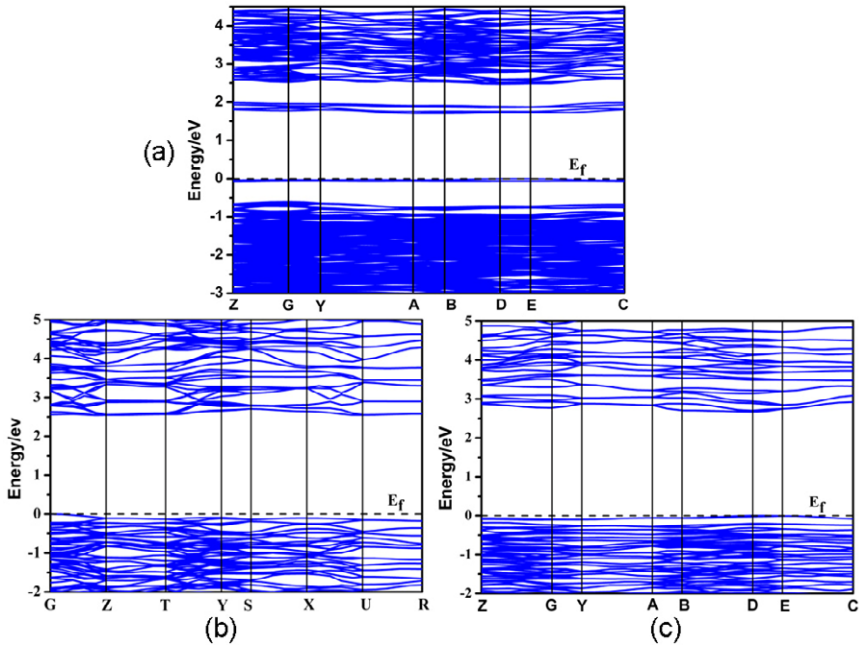


Figure S5. Band structures for the crystals $LaVO(IO_3)_5$ (a), $LaV_2O_6(IO_3)$ (b), and $LaVO_2(IO_3)_4 \cdot H_2O$ (c) (the Fermi level is set at 0 eV).

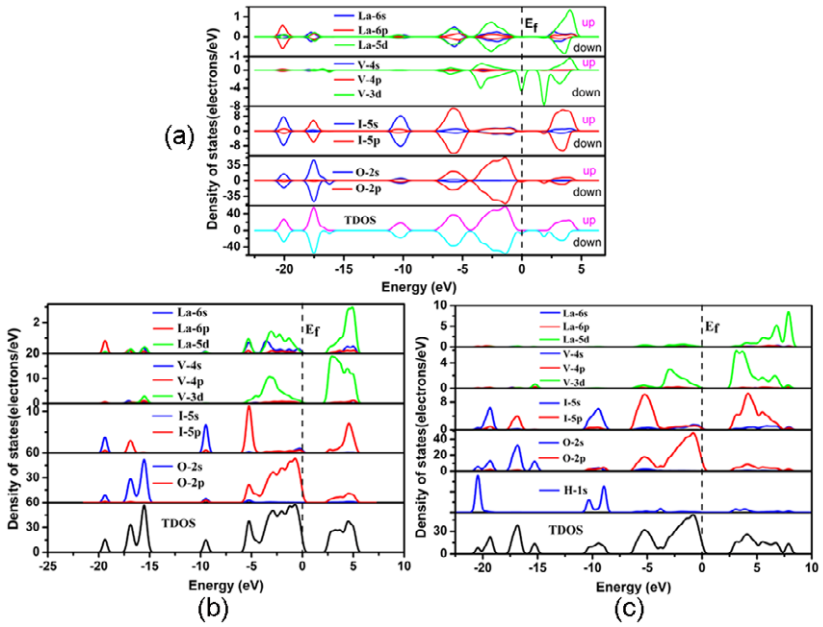


Fig. S6. The total density of states and partial density of states for $LaVO(IO_3)_5$ (a), $LaV_2O_6(IO_3)$ (b), and $LaVO_2(IO_3)_4 \cdot H_2O$ (c) (the Fermi level is set at 0 eV).