Iridate Li_8IrO_6: An Antiferromagnetic Insulator

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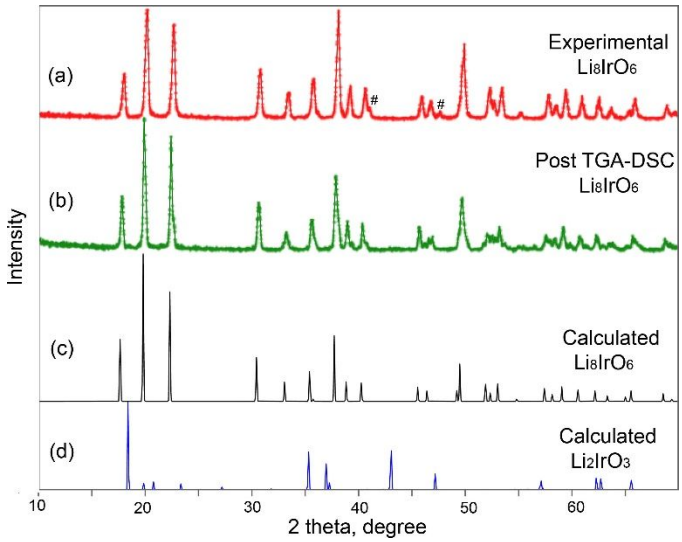

Figure S1. PXD patterns (Cu Kα, λ =1.5418 Å) of experimental Li_8IrO_6 (a), post TGA-DSC Li_8IrO_6 (b), calculated Li_8IrO_6 (c), and calculated Li_2IrO_3. Ir impurity is labeled with #.

Table S1. Summary of Rietveld refinement parameters of the second phase Li_2O. Values in parentheses indicate 1σ.

Phase	Unit cell parameters	x, y, z	Wyckoff symbol	$R_{F\text{-factor}}$	R_{bragg}	χ^2
Li_2O $Fm\bar{3}m$	$a = b = c = 4.6102(2)$ Å $\alpha = \beta = \gamma = 90°$	Li: 0.25, 0.25, 0.25 O: 0, 0, 0	Li: 4a O: 8c	8.96	15.5	1.11

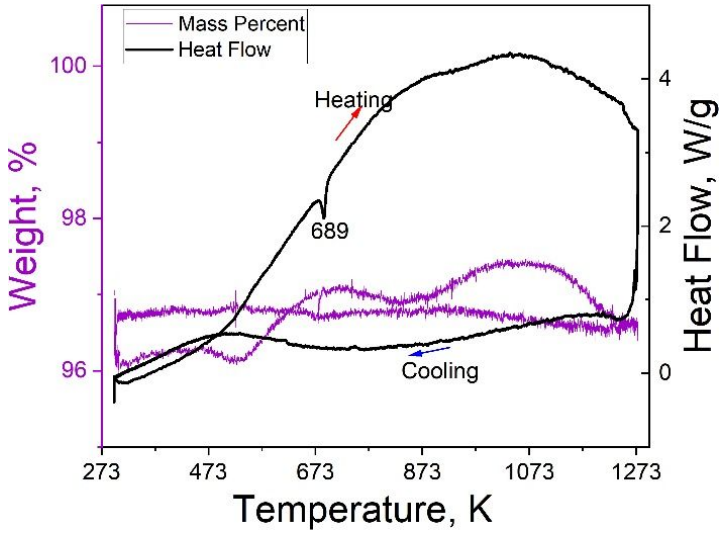

Figure S2. Temperature dependent TGA-DSC curves.

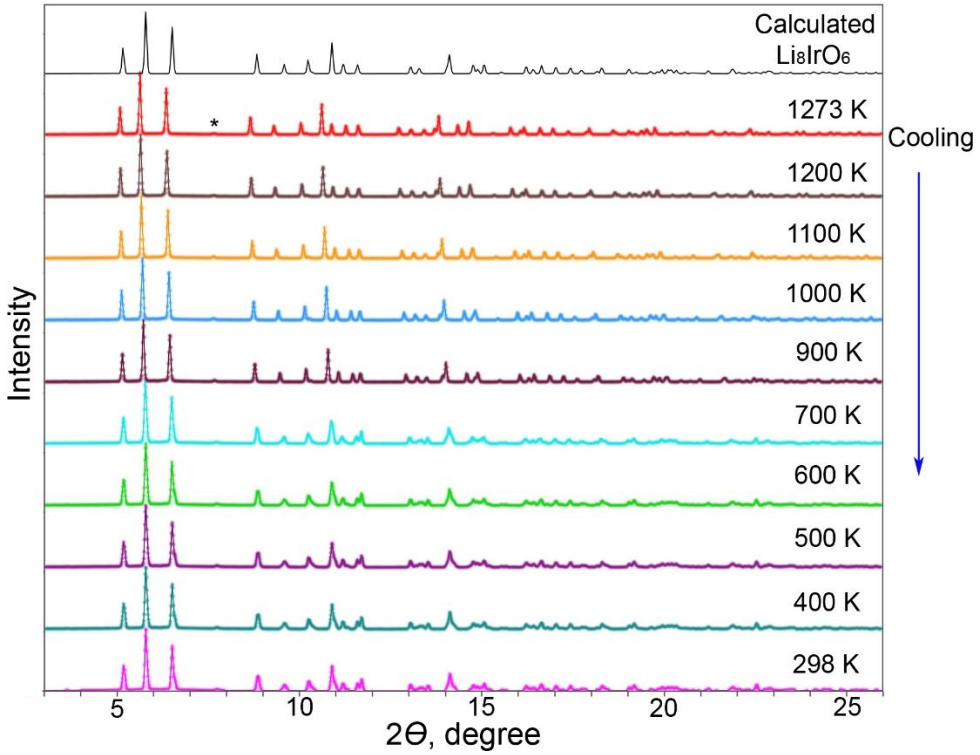

Figure S3. Experimental in-situ SPXD patterns of Li_8IrO_6 while cooling from 1273 K to 298 K. SiO_2 is marked with symbol *.

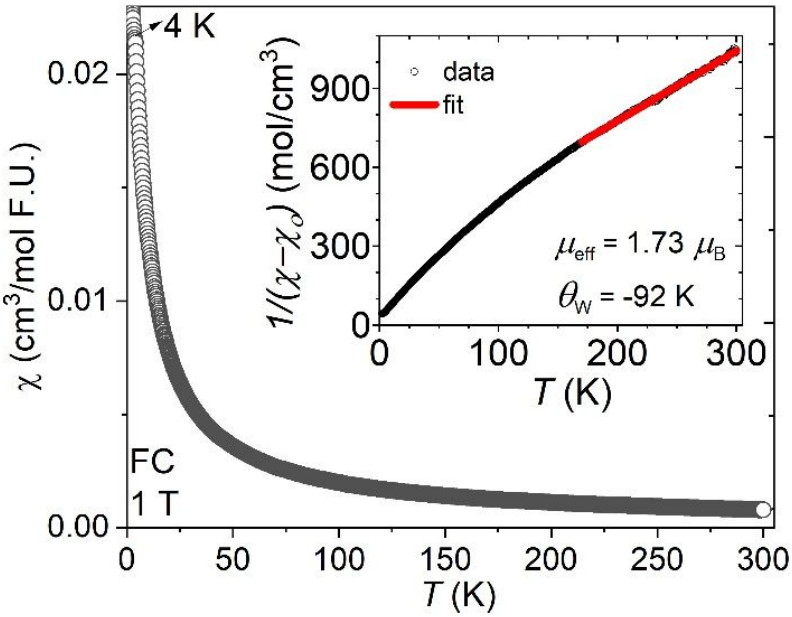

Figure S4. FC magnetic susceptibility of Li_8IrO_6 with an applied magnetic field of 1 T and inverse magnetic susceptibility fit with the $1/(\chi - \chi_o) = (T- \Theta_w)/C$ equation.

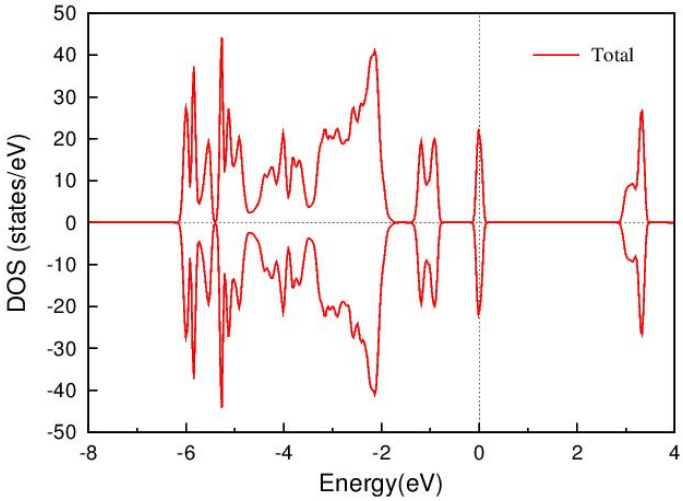

Figure S5. DOS of the NM phase with DFT GGA + SOC + U (= 4 eV) method.

Table S2. Summary of Li_8TO_6 compounds.[14-21]

Compound	***r*(T^{4+}), Å**	**Space Group**
Li_8CeO_6	0.87	$R\bar{3}$
Li_8PrO_6	0.85	$R\bar{3}$
Li_8PbO_6	0.775	$R\bar{3}$
Li_8TbO_6	0.76	$R\bar{3}$
Li_8ZrO_6	0.72	$R\bar{3}$
Li_8HfO_6	0.71	$R\bar{3}$
Li_8SnO_6	0.69	$R\bar{3}$
Li_8PtO_6	0.625	$R\bar{3}$
Li_8IrO_6	0.625	$R\bar{3}$
Li_8RuO_6	0.62	$R\bar{3}$, tetragonal?
Li_8CoO_6	0.53	$P6_3mc$
Li_8GeO_6	0.53	$P6_3mc$
Li_8SiO_6	0.4	$P6_3mc$