

Supplementary Information

Thermodynamic calculation of the conductivity of LiPON glasses and solid electrolytes

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Table S1: Entropy of known anions calculated in literature ($J \cdot mol^{-1} K^{-1}$)

Anion	Entropy ($J \cdot mol^{-1} K^{-1}$)								
	Cation charge				Anion	Cation charge			
	+1	+2	+3	+4		+1	+2	+3	+4
F¹⁻	23.0	19.7	16.7	20.9	SO₄²⁻	92.0	71.9	57.3	50.2
Cl¹⁻	40.6	33.9	28.8	33.9	CrO₄²⁻	109.5	87.8	-	-
Br¹⁻	54.3	45.6	37.6	41.8	SiO₄²⁻	79.4	57.7	37.6	33.0
I¹⁻	61.0	56.8	52.3	54.3	SiO₃²⁻	70.2	43.9	29.3	-
CN¹⁻	30.1	25.1	-	-	PO₄³⁻	100.3	71.1	50.2	-
OH¹⁻	20.9	18.8	12.5	-	HCO₂¹⁻	72.7	54.3	41.8	-
ClO¹⁻	58.5	41.8	33.4	-	H₂PO₄¹⁻	95.3	75.2	-	-

ClO₂¹⁻	80.3	71.1	58.5	-	H₂AsO₄¹⁻	104.9	87.8	-	-
ClO₃¹⁻	104.1	83.6	-	-	H¹⁻	2.1	-	-	-
ClO₄¹⁻	108.7	92.0	-	-	AlF₆³⁻	105.8	-	-	-
BrO₃¹⁻	110.8	95.7	79.4	-	AlCl₆³⁻	229.0	-	-	-
IO₃¹⁻	106.6	92.0	-	-	Al₂O₄²⁻	-	57.0	-	-
H₄IO₆¹⁻	141.7	125.4	-	-	B₂O₄²⁻		61.8	-	-
NO₂¹⁻	74.4	62.7	-	-	B₄O₇²⁻	117.6	94.8	-	-
NO₃¹⁻	90.7	74.0	62.7	58.5	B₆O₁₀²⁻	156.9	-	-	-
VO₃¹⁻	83.6	75.2	-	-	Cr₂O₄²⁻	-	84.7	-	-
MnO₄¹⁻	132.9	117.0	-	-	Fe₂O₄²⁻	-	96.3	-	-
O²⁻	10.0	2.1	2.1	4.2	MoO₄²⁻	-	84.3	-	-
S²⁻	34.3	20.9	5.4	10.5	O₂²⁻	6.4	2.5	-	-
Se²⁻	66.9	47.7	33.4	-	O₂¹⁻	76.0	-	-	-
Te²⁻	69.0	50.6	37.6	-	SiO₄⁴⁻	-	40.2	-	-
CO₃²⁻	63.5	47.7	33.4	-	TiO₃²⁻	-	51.6	-	-
SO₃²⁻	79.4	62.3	46.0	-	TiO₄⁴⁻	-	62.6	-	-
C₂O₄²⁻	92.0	74.0	58.5	-	WO₄²⁻	-	85.6	-	-

Table S2: Entropy of new anions calculated in this work ($J \cdot mol^{-1} K^{-1}$)

AlH₄¹⁻			IO₄¹⁻		
Cation	Salt	Anion	Cation	Salt	Anion
Li ¹⁺	78.7	64.1	K ¹⁺	175.7	129.3
			Na ¹⁺	163	125.8
Average		64.1	Average		127.6 ± 2.5
As³⁻			BO₂²⁻		
Ga ³⁺	64.2	24.2	Cs ¹⁺	104.4	36.5
In ³⁺	75.7	20.7	H ¹⁺	38	38
			K ¹⁺	80	33.6
			Li ¹⁺	51.5	36.9
			Na ¹⁺	73.5	36.3
			Rb ¹⁺	94.3	35
Average		22.5 ± 2.5	Average		36.1 ± 1.5
BF¹⁻			BH¹⁻		
Na ¹⁺	145.3	108.1	Li ¹⁺	75.9	61.3
			K ¹⁺	106.3	59.9

			Na ¹⁺	101.3	64.1
Average		108.1	Average		61.8 ± 2.1
BrO₄¹⁻			HF₂¹⁻		
K ¹⁺	170.1	123.7	K ¹⁺	104.3	57.9
			Na ¹⁺	90.9	53.7
			Rb ¹⁺	120.1	60.9
Average			Average		57.5 ± 3.6
SiF₆²⁻			Sb³⁻		
K ¹⁺	226	133.2	Ga ³⁺	76.1	36.1
Na ¹⁺	207.1	132.7	In ³⁺	86.2	31.2
Average		133 ± 0.4	Average		33.7 ± 3.5
HSO₄¹⁻			NH₂¹⁻		
K ¹⁺	138.1	91.7	Na ¹⁺	76.9	39.7
Na ¹⁺	113	75.8			
Average		83.8 ± 11.2	Average		39.7

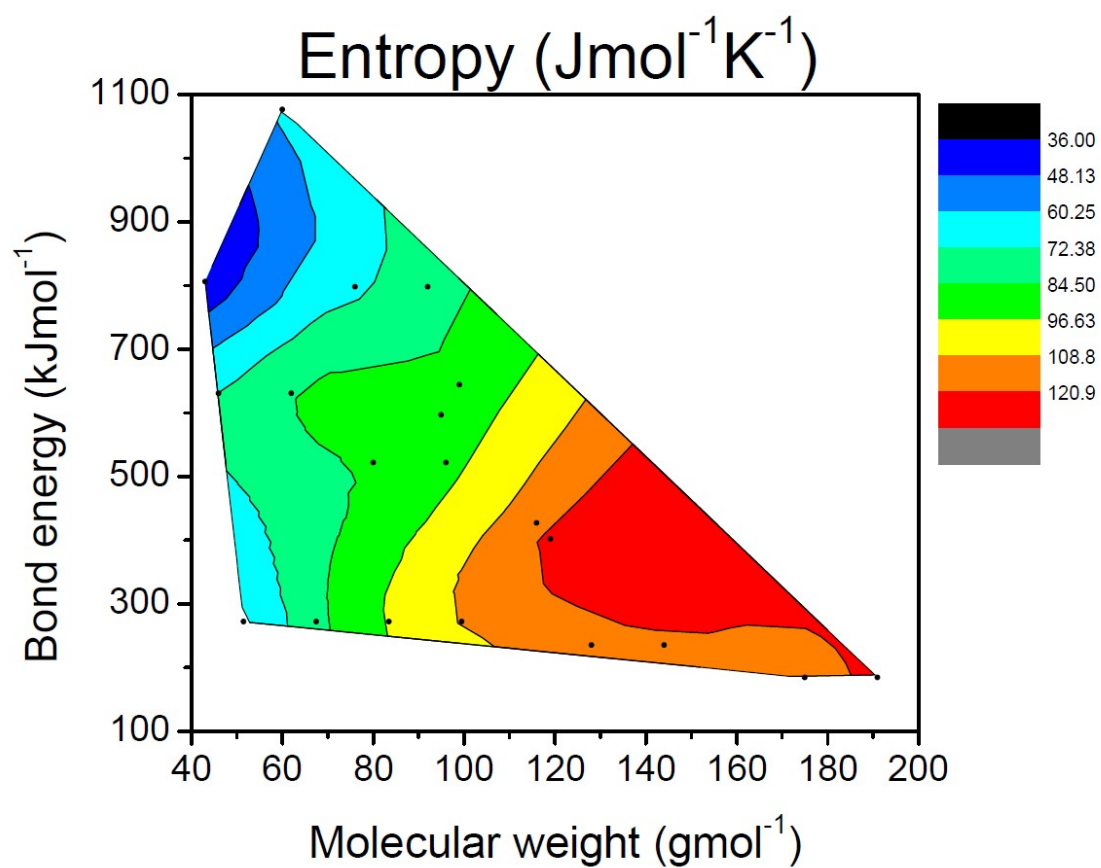


Figure S1: Entropy of different anions as a function of M_m and B_e .

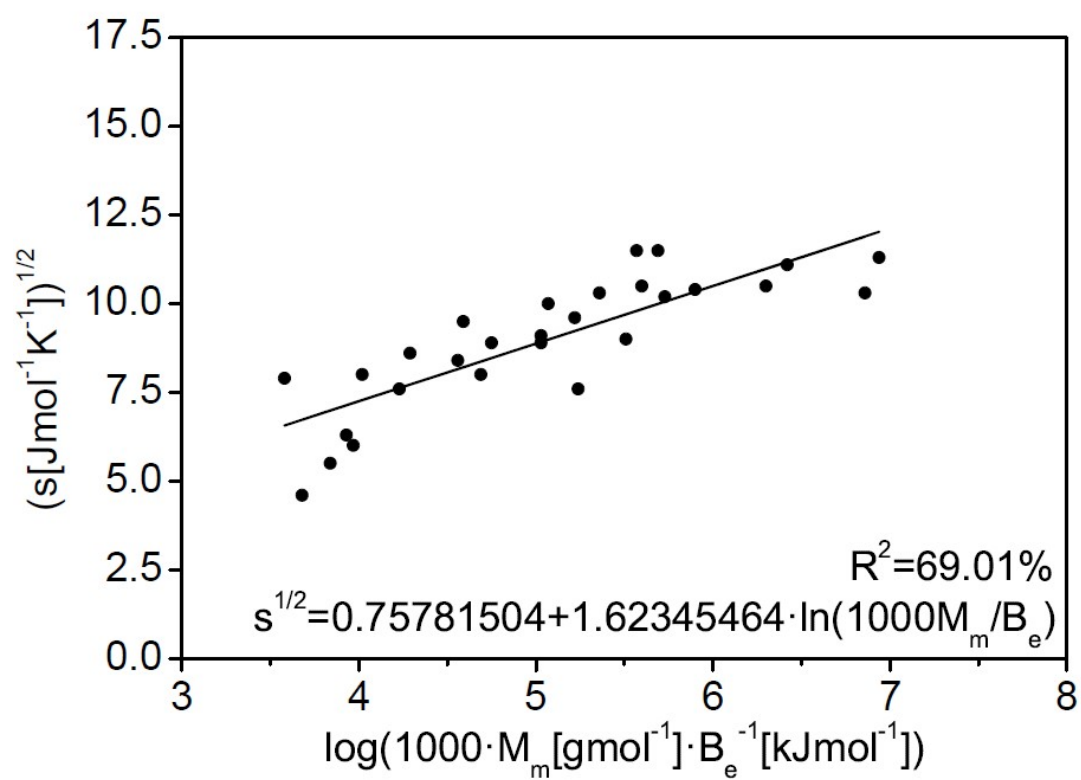


Figure S2: Plot of entropy data points and fit to Log function of molecular mass and bond energy.

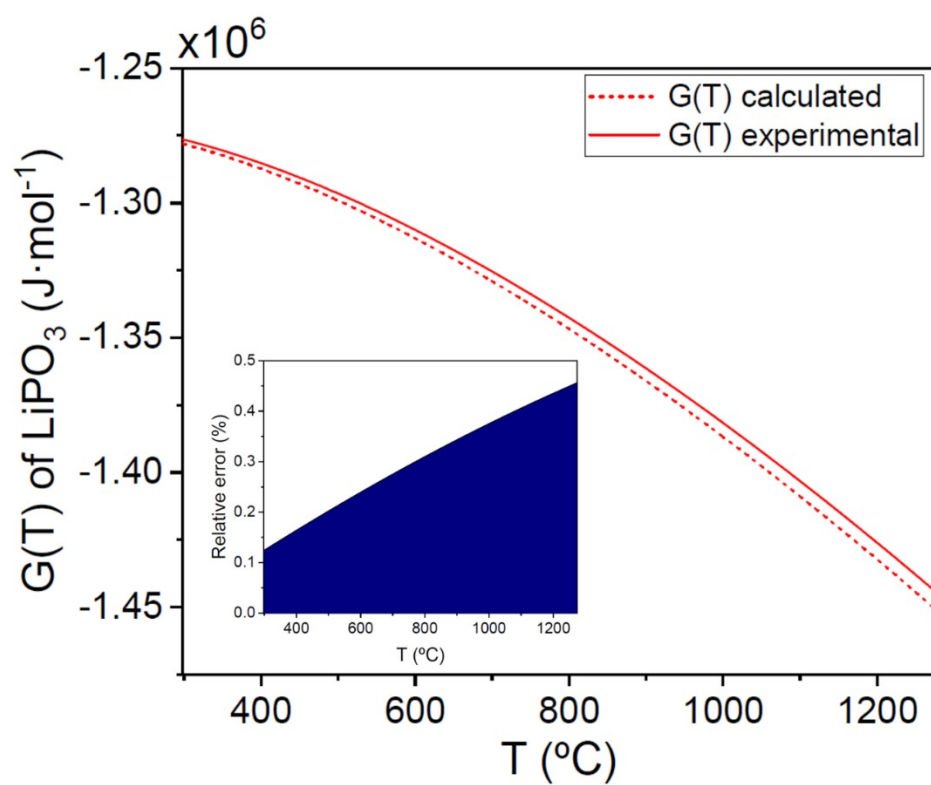


Figure S3: Calculated and experimental Gibbs free energy functions of Lithium Metaphosphate LiPO_3 .

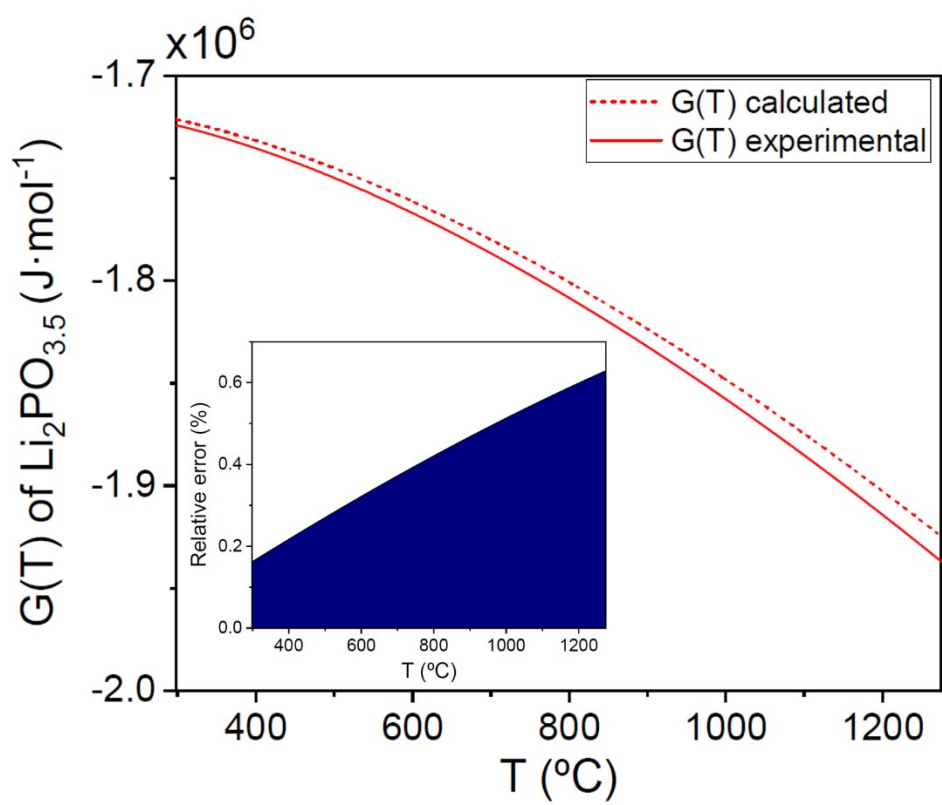


Figure S4: Calculated and experimental Gibbs free energy functions of Lithium Pyrophosphate $\text{Li}_4\text{P}_2\text{O}_7$.

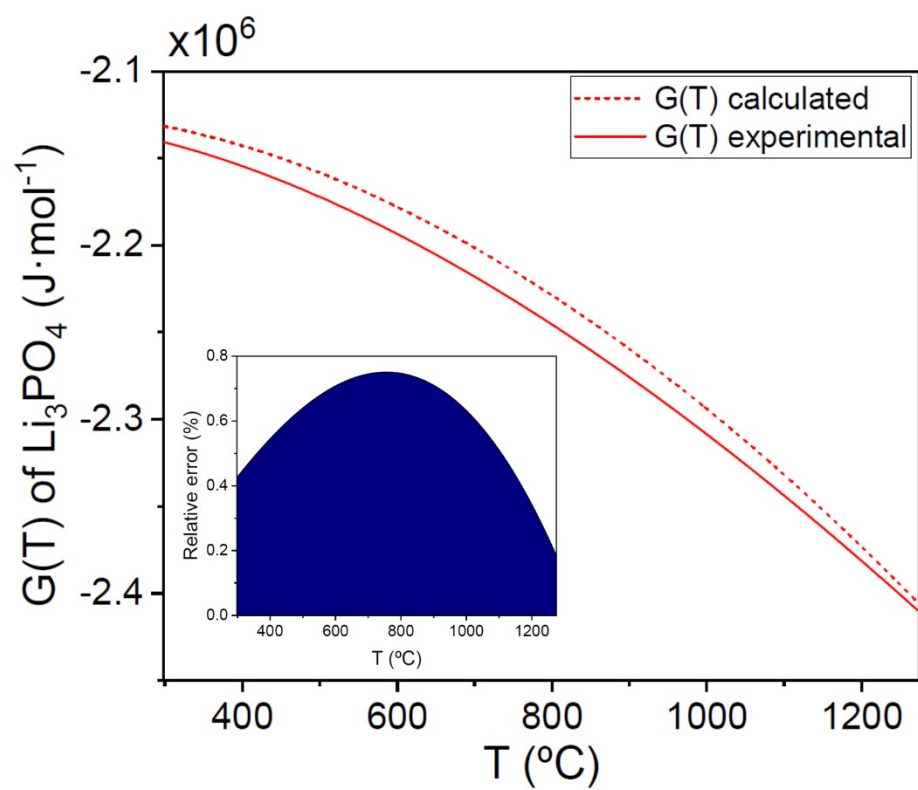


Figure S5: Calculated and experimental Gibbs free energy functions of Lithium Orthophosphate Li_3PO_4 .

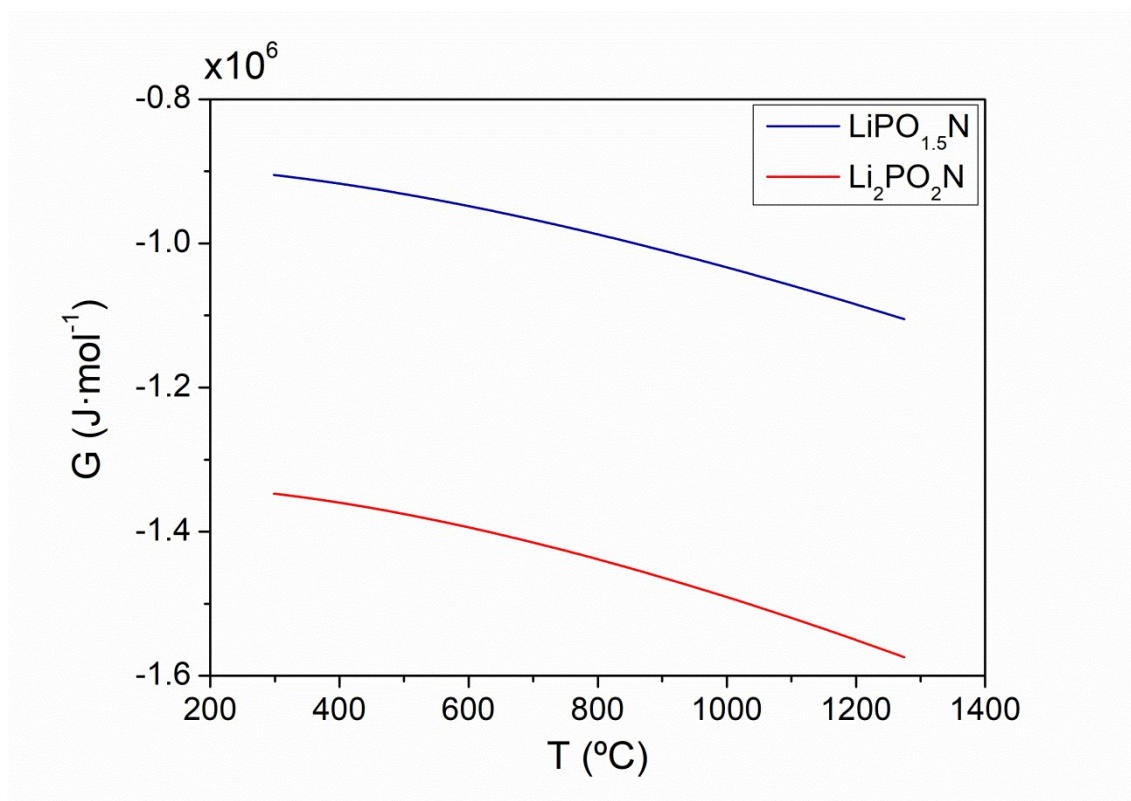


Figure S6: Calculated Gibbs free energies of $\text{LiPO}_{1.5}\text{N}$ and $\text{Li}_2\text{PO}_2\text{N}$ oxynitrides.