From the equation (1) and (2)[10], the formation energy is ΔE, the total energy of solid Li is $E_{Li}(s)$, of gas state O_2 is $E_{O_2}(g)$, of rhombic sulfur is $E_{S_6}(s)$, the calculated theoretical and experimental data are listed in table S1. The formation energy for Li_2O_2, LiO_2 is lower than the previous work due to temperature effect to a certain extent. The low formation energy of Li_2S indicates that Li_2S is easily reproduced during the discharge process.

$$\Delta E = E_{Li_xO_y}(s) - xE_{Li}(s) - \frac{y}{2}E_{O_2}(g) \quad (1)$$

$$\Delta E = E_{Li_2S}(s) - 2E_{Li}(s) - \frac{1}{6}E_{S_6}(g) \quad (2)$$

Table S1 Predicted standard formation energy and total energies at zero temperature and their comparisons with available experimental and theoretical data at 298.15K

	Li	O_2	S_6	Li_4O_4	LiO_2	Li_2S
Total energy	-194.8	-867.52	-1823.86	-2532.59	-1063.76	-700.17
Formation energy(ΔE)				-9.175 (-6.569[10],-6.557[S1])	-1.44 (-3.272[10],-2.689[S2])	-6.59

*The Computational methods of Li, O_2, S_6 are consistent with Li_2O_2, LiO_2, and Li_2S.

Table S2 Predicted bandgaps and their comparisons with available theoretical data

Method type	Bandgaps （eV）	
	Li_2O_2	Li_2S
GGA-PBE	1.894	3.398
GGA-WC	1.934	3.212
HES06	5.040	4.069
GGA-RPBE(PBE)	1.88(1.99)[23,24]	
GGA-PBE, and vdW-DF		3.46[25]

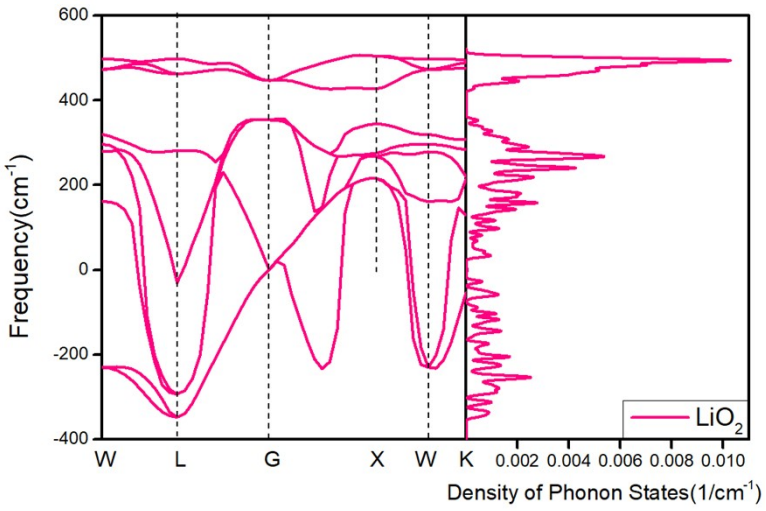

Fig. S1 The phonon dispersion of the LiO_2

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