Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Formation of Li_3O_4 nano particles in the discharge products of non-aqueous lithium-oxygen batteries leads to lower charge voltage

Supporting Information

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Table. S1 Lattice constant of LiO_2 (*Pnnm*)

	Zhuravlev et al. [1]	Seriani [2]	Lau et al. [3]	Kang et al [4]	Our work	Experiment by Bakulina et al. [5]
a (Å)	3.99	3.90	3.95	4.01	3.94	5.91
b (Å)	4.88	4.64	4.94	4.80	4.92	4.94
c (Å)	2.96	2.81	2.96	3.03	2.96	4.38
Note	GGA	GGA	GGA	HSE	GGA	

Table. S2 Lattice constant of Li_2O_2 and Li_3O_4

	a (Å)	b (Å)	c (Å)
Li_2O_2 (*P6₃/mmc*)	3.14	3.14	7.65
Li_3O_4 ($P\bar{6}m2$)	3.13	3.13	7.38

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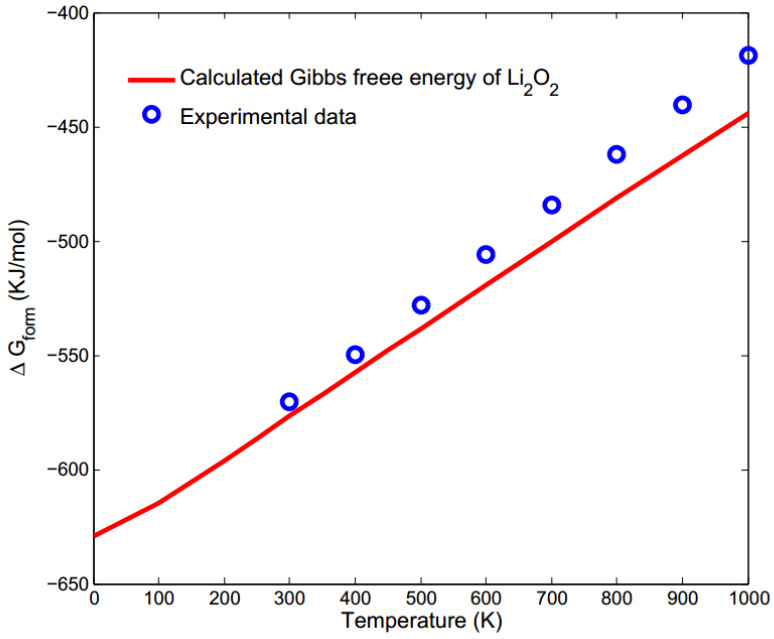
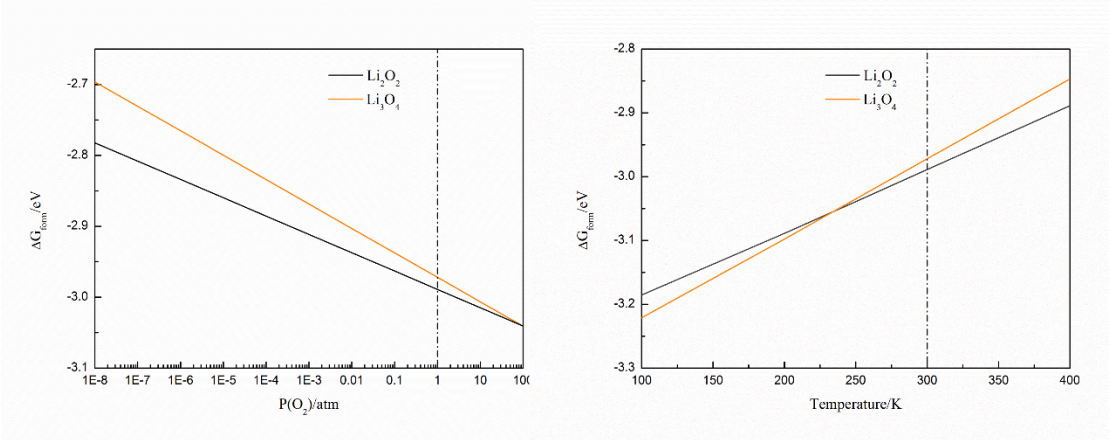


Fig. S1 Calculated Gibbs free energy of Li_2O_2 compared with experimental values [6]



(a) (b)

Fig. S2 Formation Gibbs free energy of Li_2O_2 and Li_3O_4 under (a) different oxygen pressures when T = 300 K (b) different temperatures when P (O_2) = 1 atm

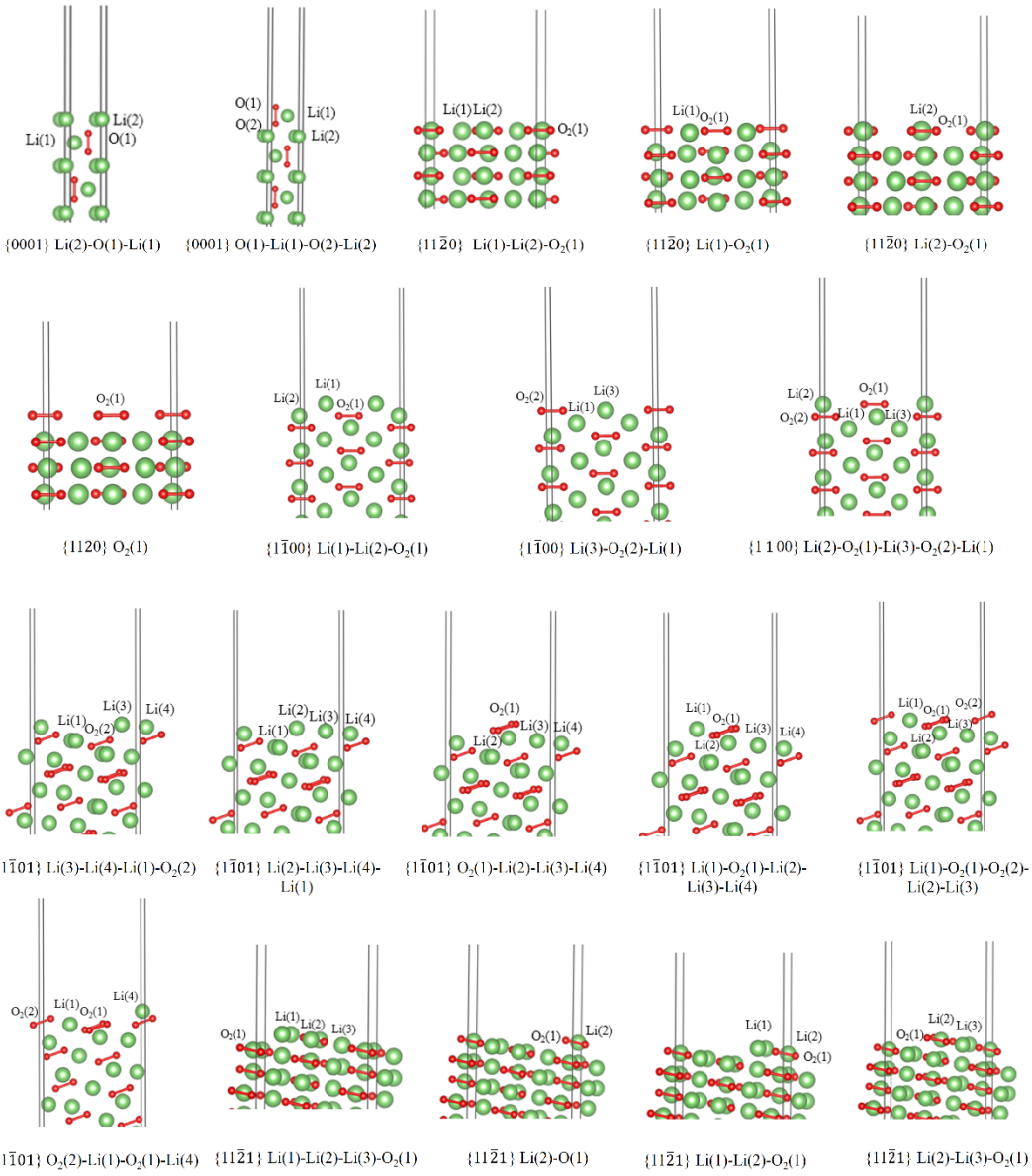
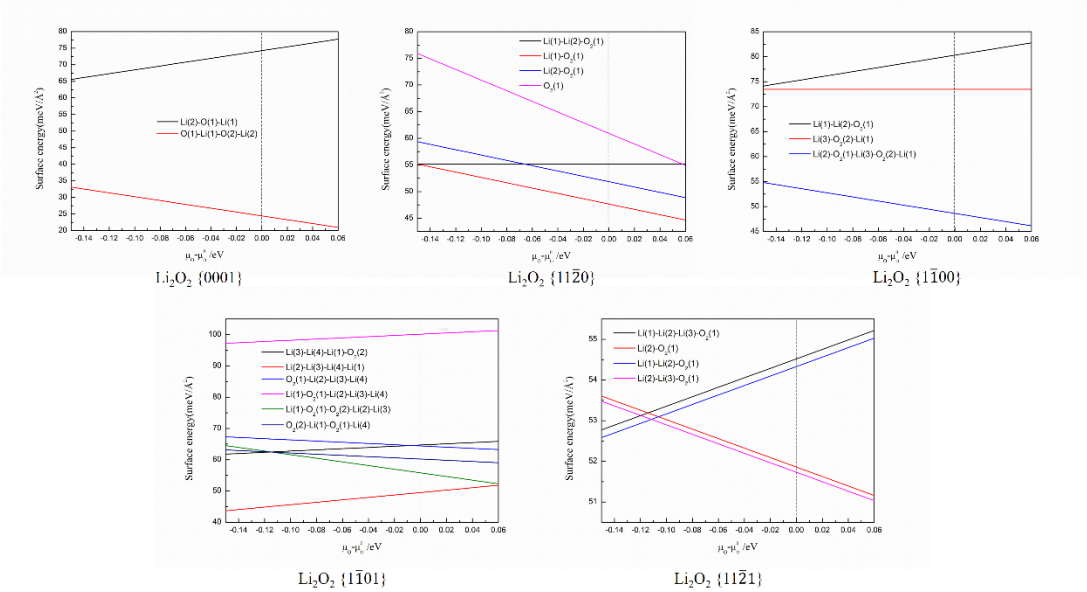


Fig. S3 Structures of terminations considered in the calculation of Li_2O_2 surface energies



Li_2O_2 {0001} Li_2O_2 {11$\bar{2}$0} Li_2O_2 {1$\bar{1}$00}

Li_2O_2 {1$\bar{1}$01} Li_2O_2 {11$\bar{2}$1}

Fig. S4 Surface energies of different terminations of Li_2O_2 as a function of oxygen chemical potential

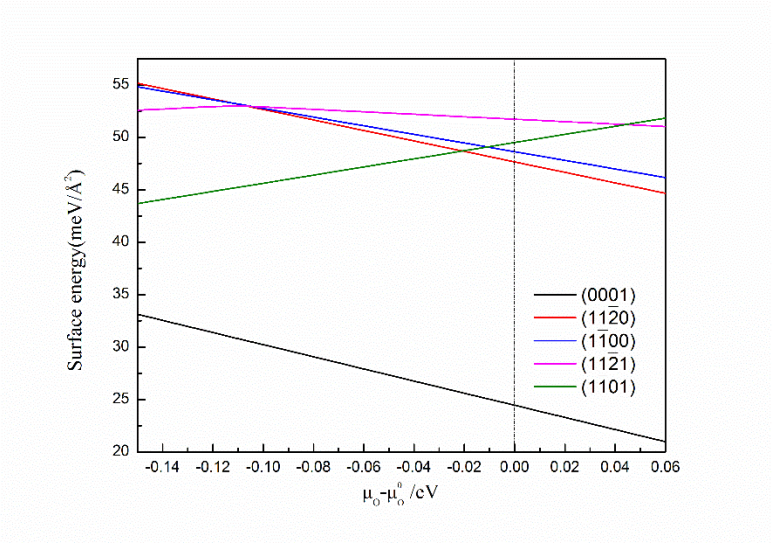


Fig. S5 Surface energies of different orientations of Li_2O_2 as a function of oxygen chemical potential

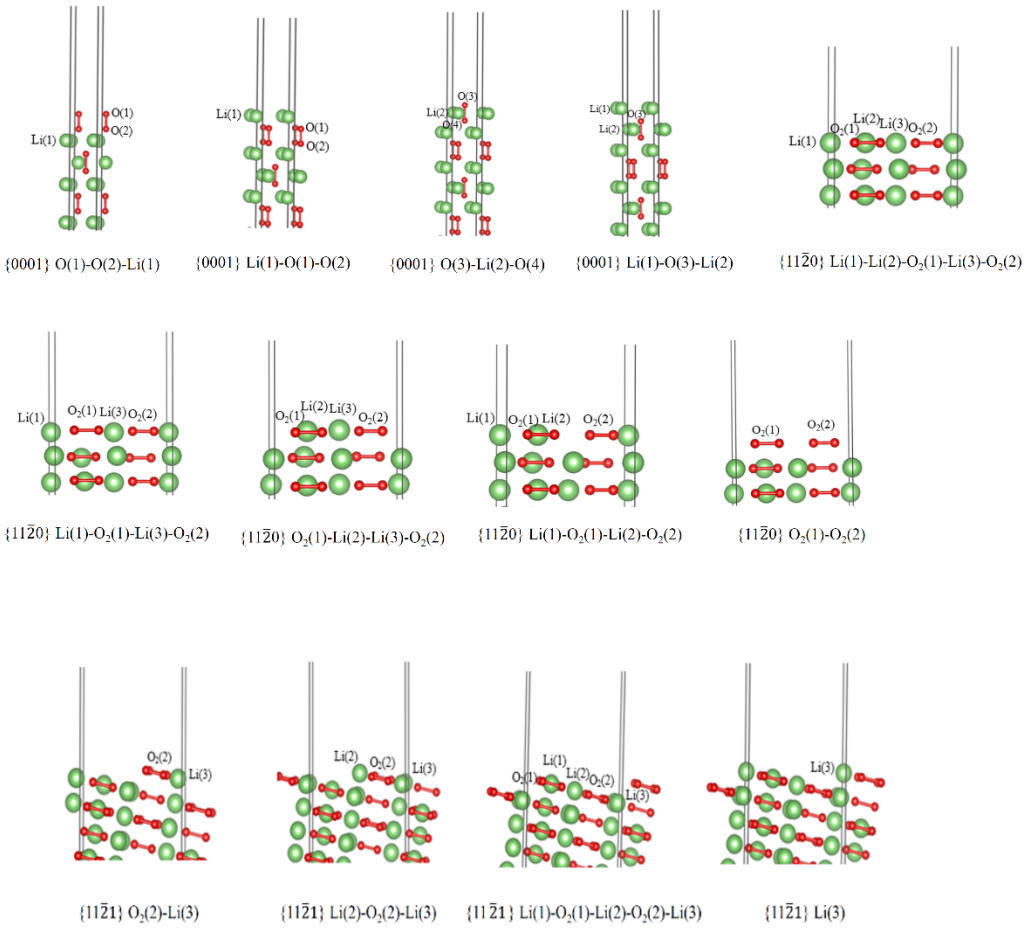
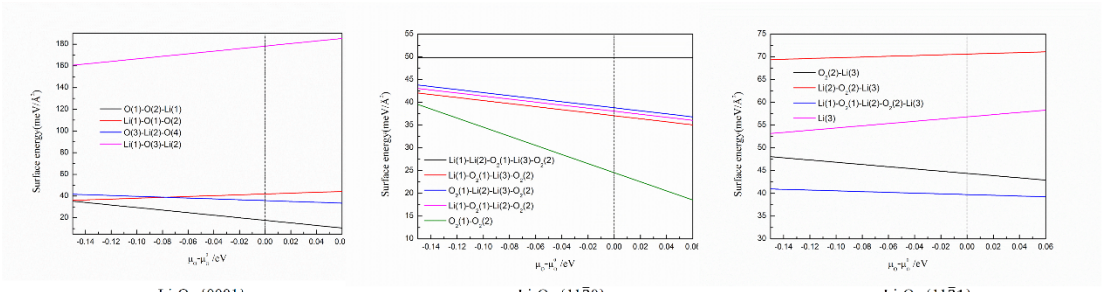


Fig. S6 Structures of terminations considered in the calculation of Li_3O_4 surface energies



Li_3O_4 {0001} Li_3O_4 {11$\bar{2}$0} Li_3O_4 {11$\bar{2}$1}

Fig. S7 Surface energies of different terminations of Li_3O_4 as a function of oxygen chemical potential

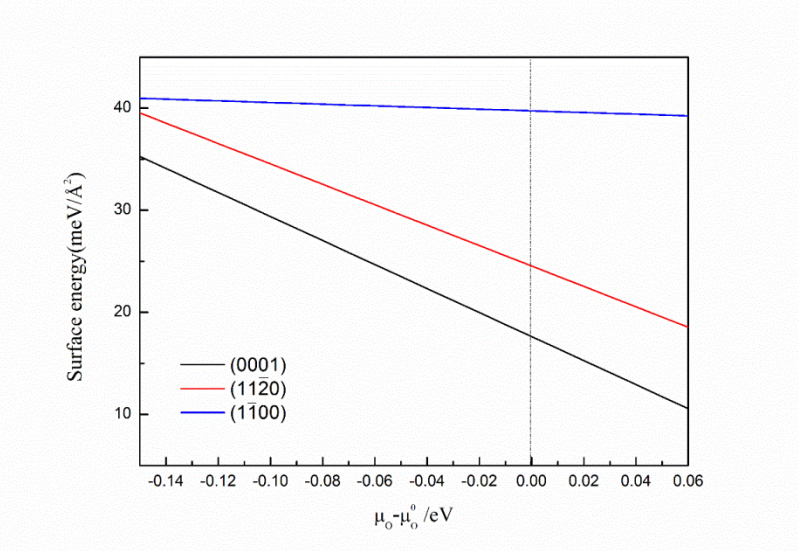


Fig. S8 Surface energies of different orientations of Li_3O_4 as a function of oxygen chemical potential

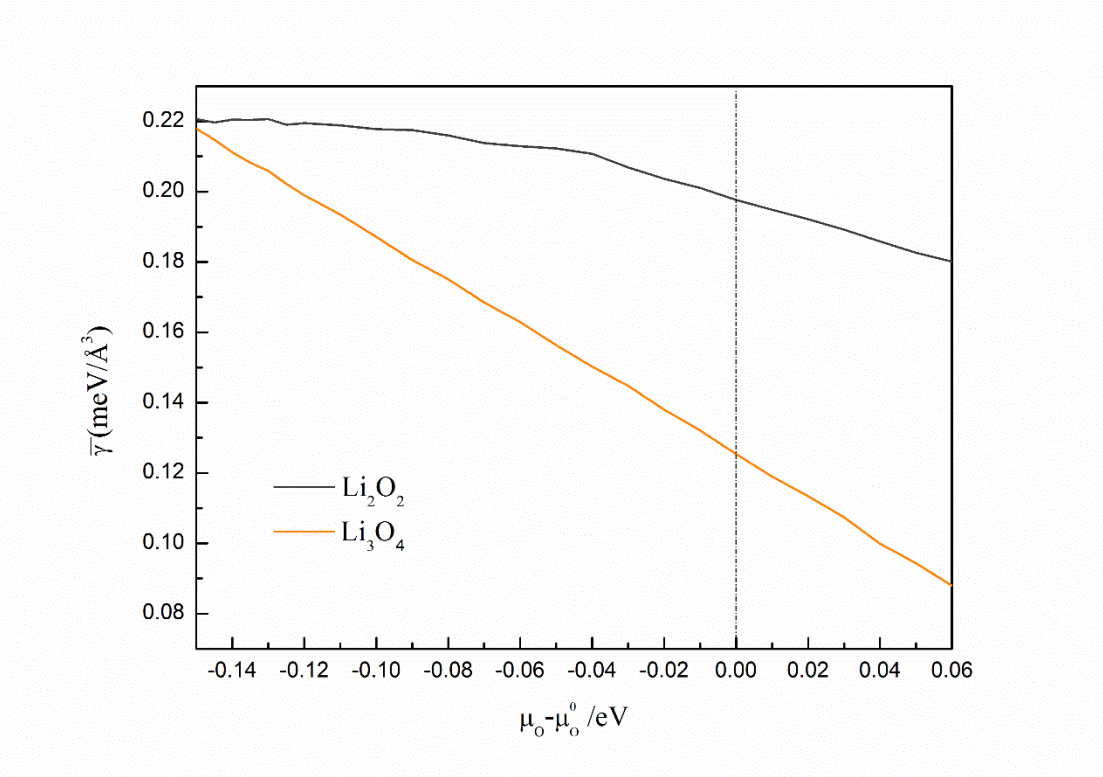


Fig. S9 The normalized surface energies of Li_3O_4 and Li_2O_2 as a function of oxygen chemical potential

References

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