

Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A. This journal is © The Royal Society of Chemistry 2022

Electronic Supplementary Information

## **Lattice distortion derived catalytic degradation in multi-oxide**

### **cathode catalyst for Li-oxygen batteries**

Ruwei Liu<sup>a</sup>, Yiming Fu<sup>b</sup>, Guoliang Zhang<sup>a</sup>, Liang Guo<sup>a</sup>, Ruonan Yang<sup>a</sup>, Xiuqi Zhang<sup>a</sup>, Qing Zhu<sup>\*c</sup> and Feng Dang<sup>\*a</sup>

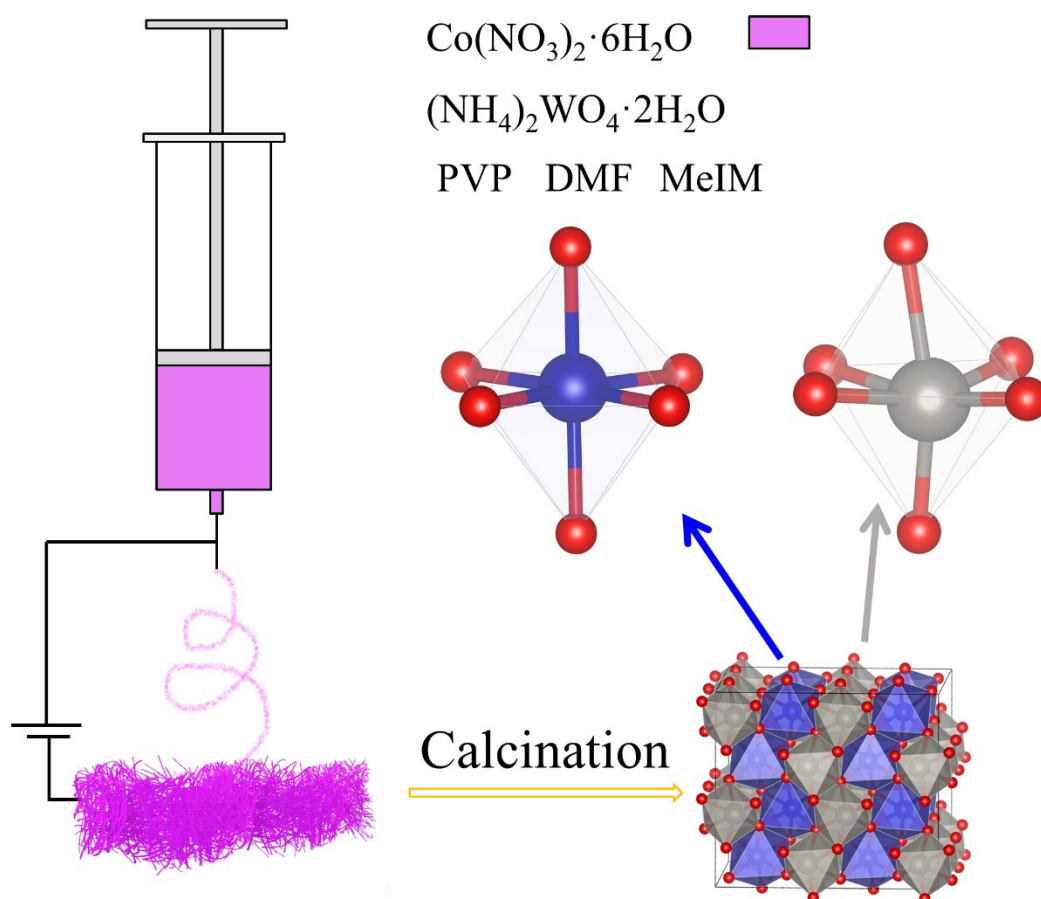
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<sup>a</sup> Key Laboratory for Liquid-Solid Structural Evolution and Processing of Materials (Ministry of Education), Shandong University, 17923 Jingshi Road, Jinan, 250061, Shandong Province, P.R.China. E-mail: dangfeng@sdu.edu.cn.

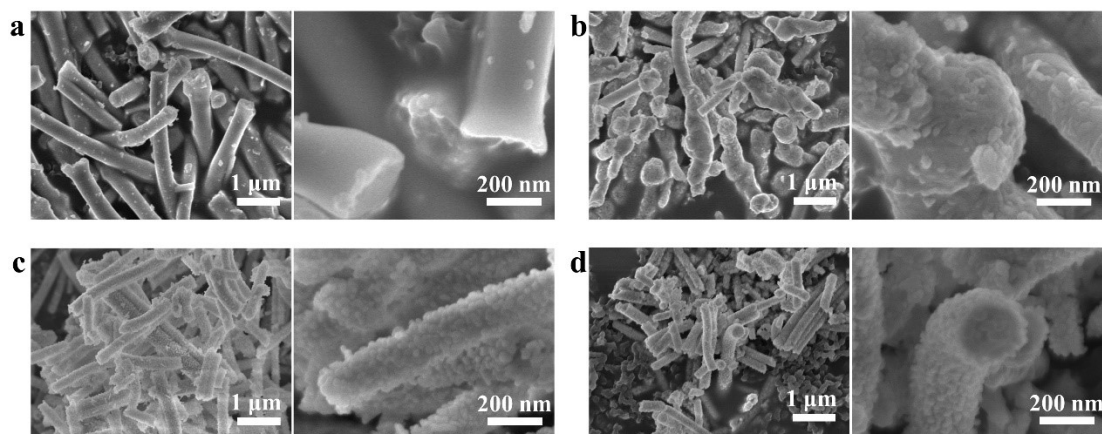
<sup>b</sup> School of Life Sciences, Qilu Normal University, Jinan, 250200, Shandong Province, P.R. China. E-mail: 20152789@qlnu.edu.cn

<sup>c</sup> Shandong Institute of Innovation and Development, Jinan, 250101, Shandong Province, P.R. China. E-mail: zhuqing0109@163.com.

*Chemical reagents:* All the chemical required for the synthesis, including Polyvinylpyrrolidone (PVP, Macklin, China), N, N-dimethylformamide solvent (DMF) (99.5%, Sinopharm, China), acetate (99.5%, Aladdin, China), 2-Methylimidazole (MeIM) (98%, Aladdin, China), methanol(99.5%, Sinopharm, China), Cobalt(II) acetate tetrahydrate( $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ ), ammonium metatungstate hydrate( $(\text{NH}_4)_6\text{H}_2\text{W}_{12}\text{O}_{40} \cdot x\text{H}_2\text{O}$ , 99.95%, Aladdin, China) and deionized water were used as received without further purification.

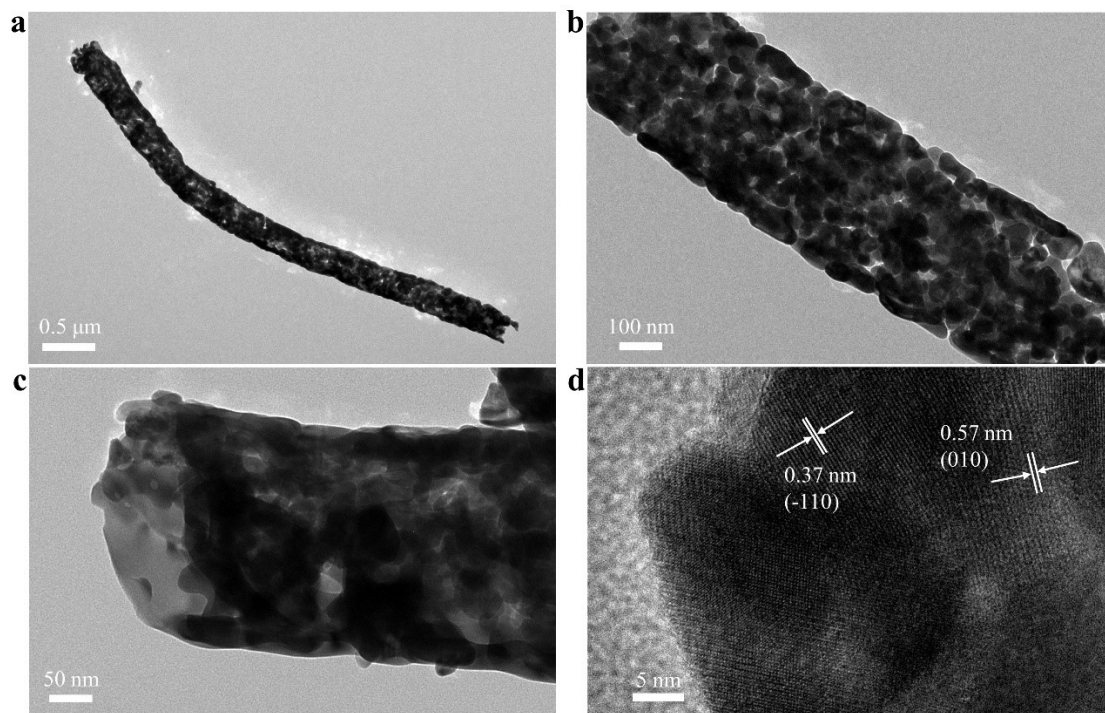


**Figure S1.** Schematic illustration of the preparation procedure of  $\text{CoWO}_4$  nanofibers.



**Figure S2.** SEM images of a)  $\text{CoWO}_4$ , b)  $\text{CoWO}_5$ , c)  $\text{CoWO}_6$  and d)  $\text{CoWO}_7$ .





**Figure S3.** HRTEM images of CoWO-7.

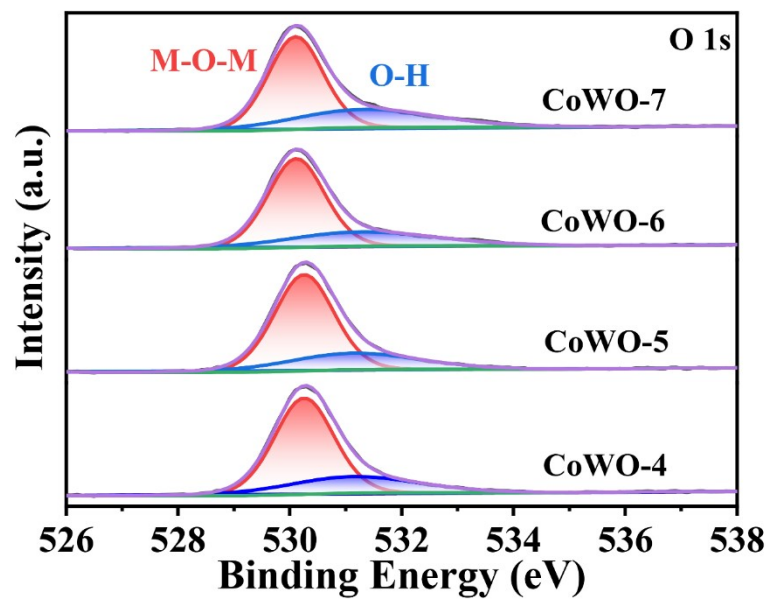
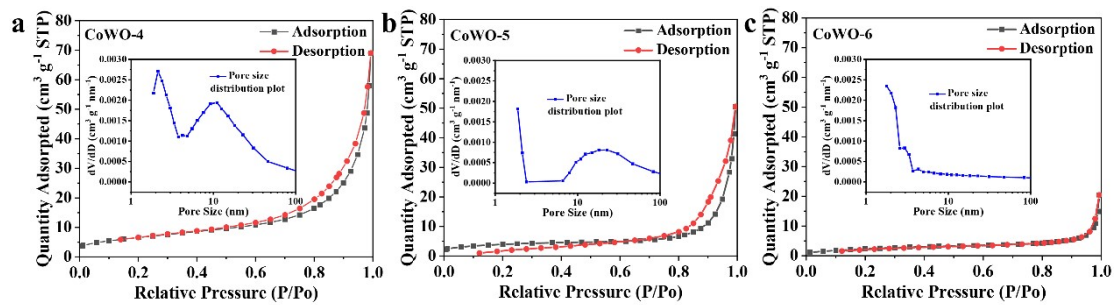
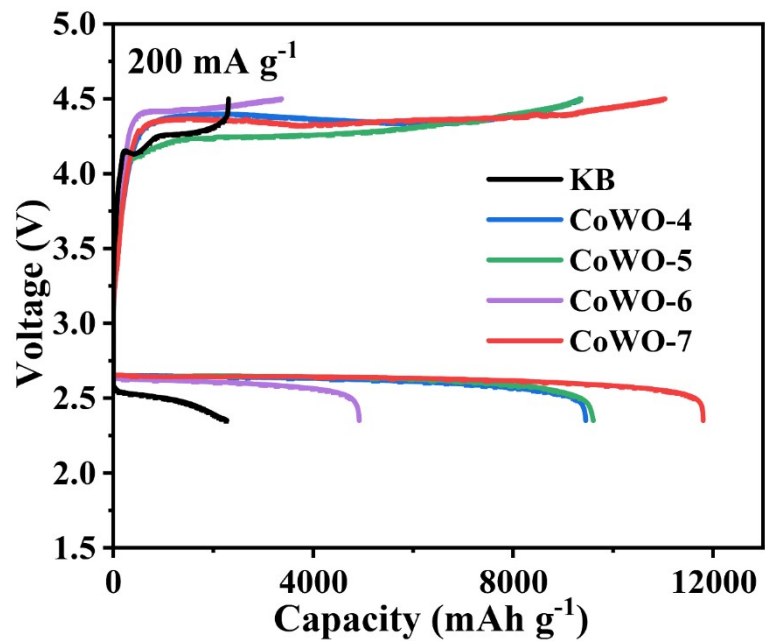


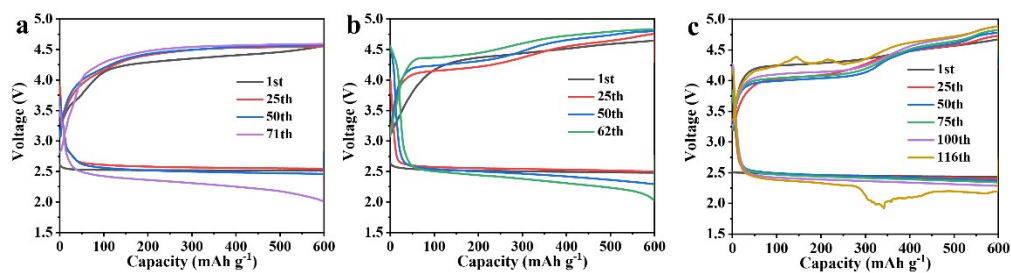
Figure S4. XPS spectra of O 1s.



**Figure S5.** BET profiles of a) CoWO-4, b) CoWO-5 and c) CoWO-6.



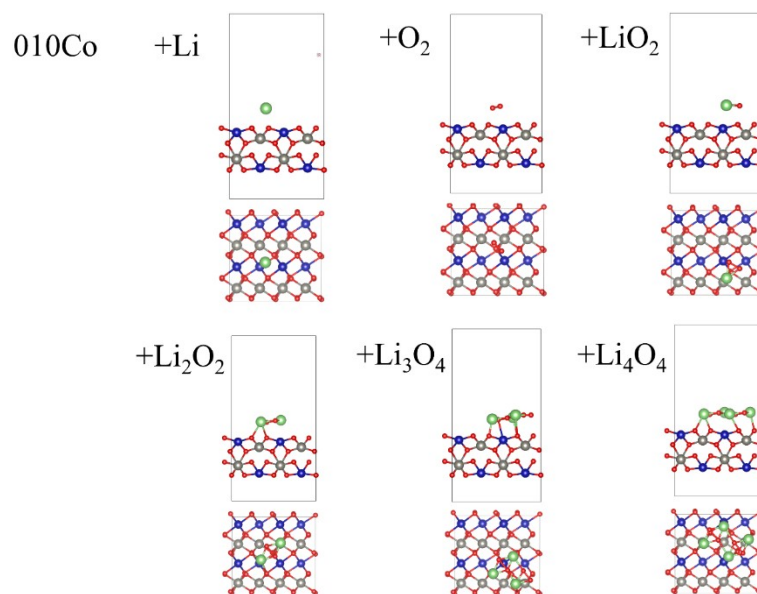
**Figure S6.** Specific capacity of Li-O<sub>2</sub> batteries with different electrodes at a current density of 200 mA g<sup>-1</sup>.



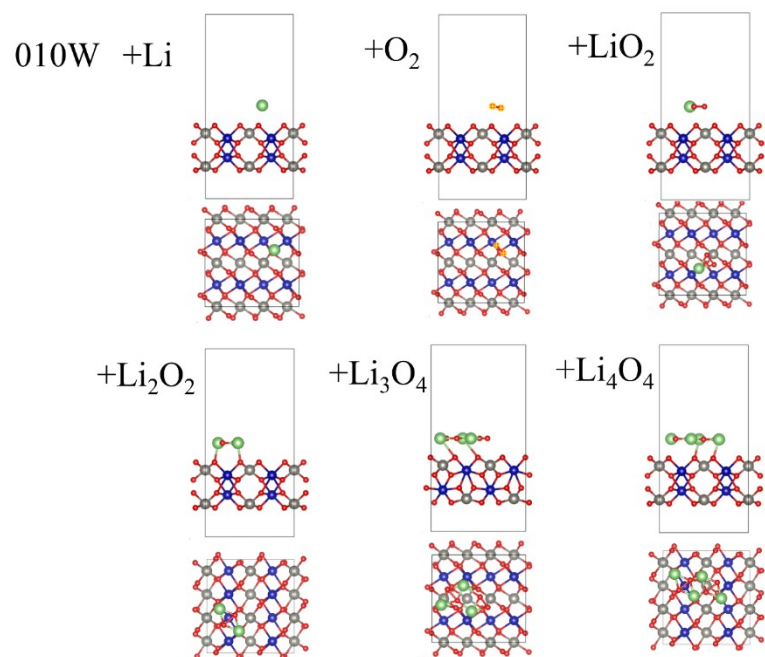
**Figure S7.** Selected discharge/charge curves with voltages of  $\text{CoWO}_4$  samples within an upper-limited specific capacity of  $600 \text{ mAh g}^{-1}$  at a current density of  $1000 \text{ mA g}^{-1}$ : a) CoWO-4, b) CoWO-5 and c) CoWO-6.



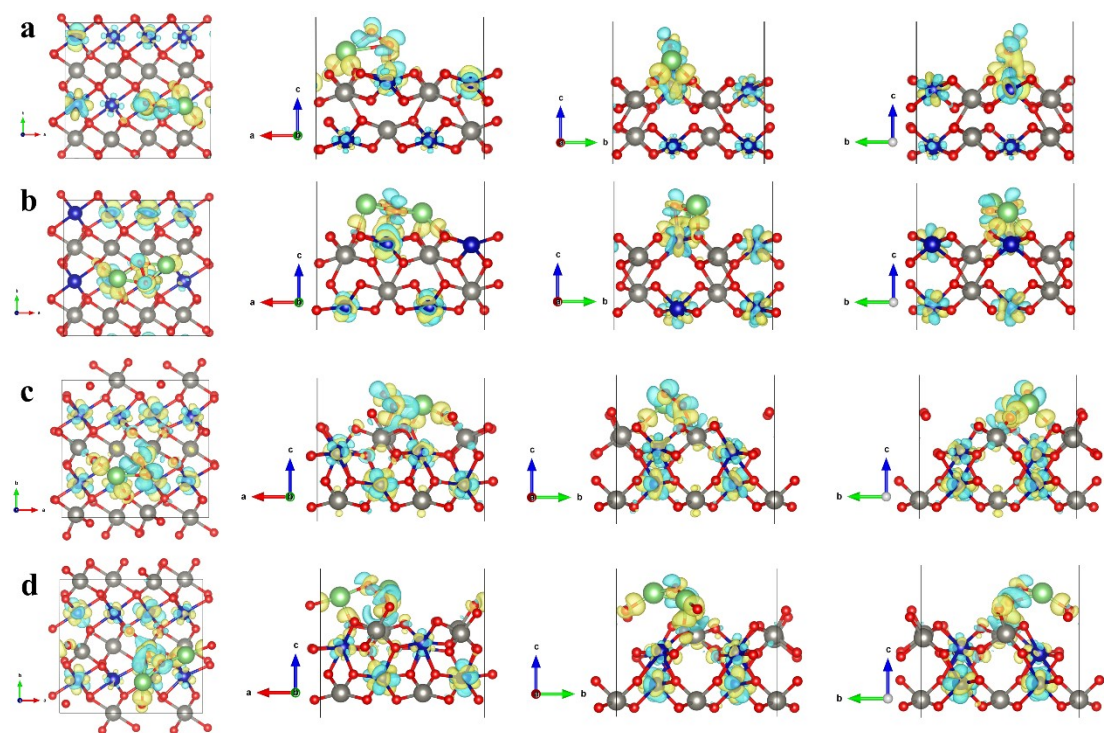
DFT calculation:



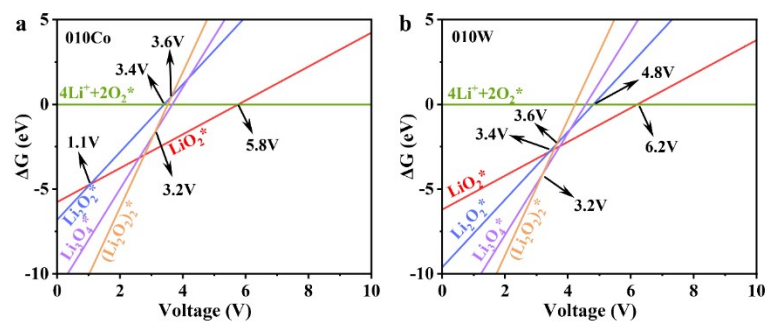
**Figure S8.** The most stable structure of different adsorbed species on 010Co surface.



**Figure S9.** The most stable structure of different adsorbed species on 010W surface.



**Figure S10.** Charge density difference of  $\text{LiO}_2$  and  $\text{Li}_2\text{O}_2$  adsorbates on 010 surfaces from different directions. (a)  $010\text{Co} + \text{LiO}_2$ , (b)  $010\text{Co} + \text{Li}_2\text{O}_2$ , (c)  $010\text{W} + \text{LiO}_2$ , and (d)  $010\text{W} + \text{Li}_2\text{O}_2$ .



**Figure S11.** Phase diagrams of the cathode reaction on a) 010Co and b) 010W facets.

**Table S1.** Result of BET of CoWO<sub>4</sub> samples.

<b>Sample</b>	<b>Surface area [m<sup>2</sup> g<sup>-1</sup>]</b>	<b>Pore volume [cm<sup>3</sup> g<sup>-1</sup>]</b>	<b>Pore size [nm]</b>
CoWO-4	23.8414	0.035916	37.8266
CoWO-5	13.3943	0.078211	35.0059
CoWO-6	8.8363	0.036583	33.4177
CoWO-7	6.3868	0.017345	17.5010

**Table S2.** Comparison of surface energy of low-Miller-index facets.

<b>Surface</b>	<b>Surface energy (J m<sup>-2</sup>)</b>
001	0.9072
010	0.4925
010	1.3533
100	3.0056
011	2.1803
101	2.5211
110	1.331
111	2.4914
020	1.174
200	3.0049
-111	3.4629

**Table S3.** The calculated adsorption energy ( $E_{\text{ads}}$ ) of different adsorbed species on different planes and corresponding Bader charge analysis result ( $\Delta Q$ ) and distance between the adsorbed species and surface of substrates.

<b>010Co</b>	<b><math>E_{\text{ads}}(\text{eV})</math></b>	<b><math>\Delta Q(\text{surface})</math></b>	<b><math>\Delta Q(\text{adsorbate})</math></b>	<b><math>R(\text{\AA})</math></b>
Li	-0.87528	0.90332	-0.90905	1.49520
O <sub>2</sub>	0.03874	-0.00440	0.00440	3.17919
LiO <sub>2</sub>	-3.06703	0.24940	-0.24940	1.81641
Li <sub>2</sub> O <sub>2</sub>	-2.64276	0.45639	-0.45639	1.63198
Li <sub>3</sub> O <sub>4</sub>	-2.35432	0.41179	-0.41179	2.16879
Li <sub>4</sub> O <sub>4</sub>	-3.77246	0.63593	-0.63593	1.91556
<b>010W</b>	<b><math>E_{\text{ads}}(\text{eV})</math></b>	<b><math>\Delta Q(\text{surface})</math></b>	<b><math>\Delta Q(\text{adsorbate})</math></b>	<b><math>R(\text{\AA})</math></b>
Li	-5.91735	0.91576	-0.91577	0.76442
O <sub>2</sub>	-2.03282	-0.00328	0.00327	2.86156
LiO <sub>2</sub>	-3.50619	0.28006	-0.28007	1.26172
Li <sub>2</sub> O <sub>2</sub>	-5.44270	0.49621	-0.49621	1.48843
Li <sub>3</sub> O <sub>4</sub>	-5.03443	0.62797	-0.62797	1.42463
Li <sub>4</sub> O <sub>4</sub>	-6.57695	0.83627	-0.83628	1.52208