RuO_2 Monolayer: A Promising Bi-Functional Catalytic Material for Non-Aqueous Lithium-Oxygen Batteries

Supporting Information

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Table. S1 Optimized lattice parameters of Li_2O_2, RuO_2 monolayer and rutile RuO_2

	a (Å)	b (Å)	c (Å)
Li_2O_2 (*P6₃/mmc*)	3.14	3.14	7.65
RuO_2 monolayer ($R\bar{3}m$)	2.93	2.93	--
Rutile RuO_2 (*P4₂/mnm*)	4.52	4.52	3.11

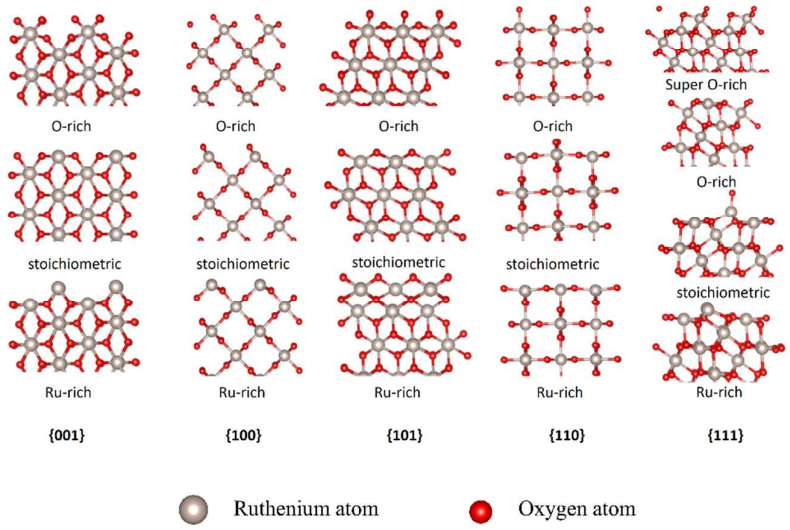

Fig. S1 The orientations and terminations of rutile RuO_2 considered for the Wulff construction.

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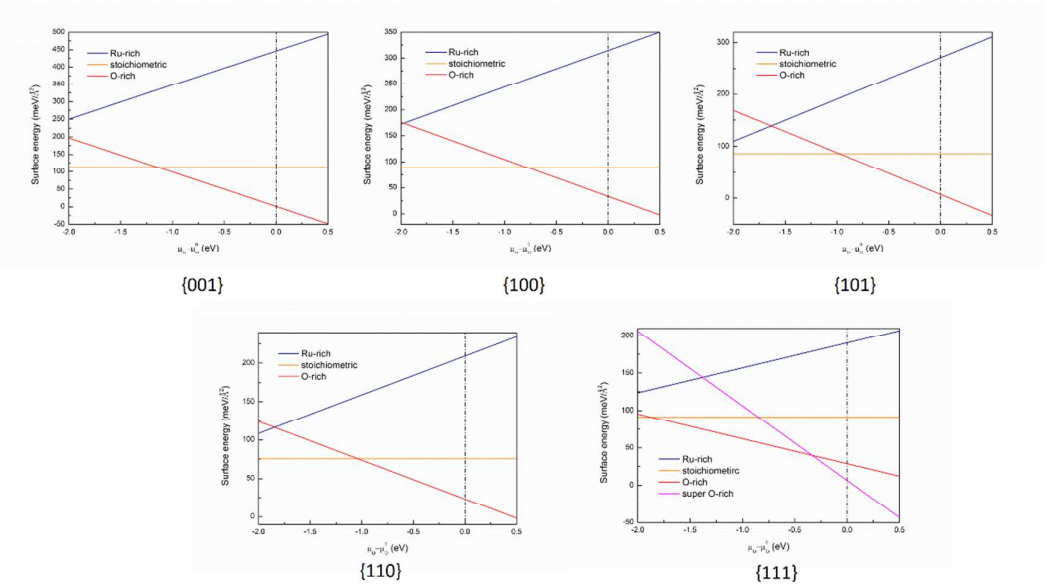

Fig. S2 Surface energies of different orientations and terminations of rutile RuO_2 under different oxygen chemical potentials

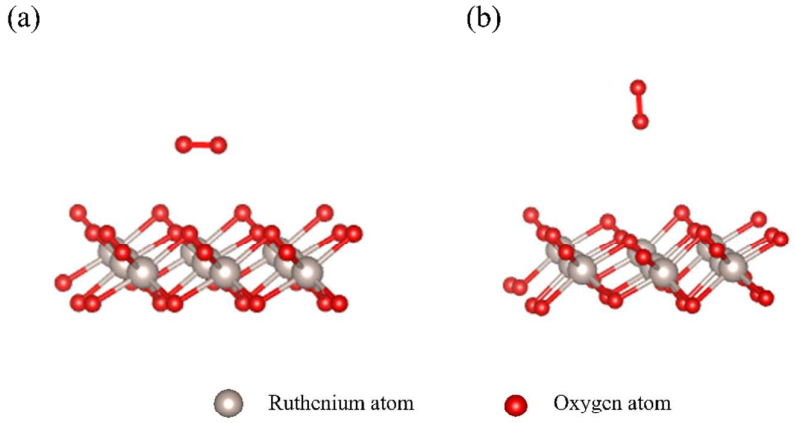

Fig. S3 Optimized geometry for oxygen molecular adsorbed onto the surface of RuO_2 monolayer. Two initial geometries were considered (a and b). The oxygen-oxygen bond lengths in both cases are 1.22Å (The bond length for free oxygen molecular is 1.21 Å).

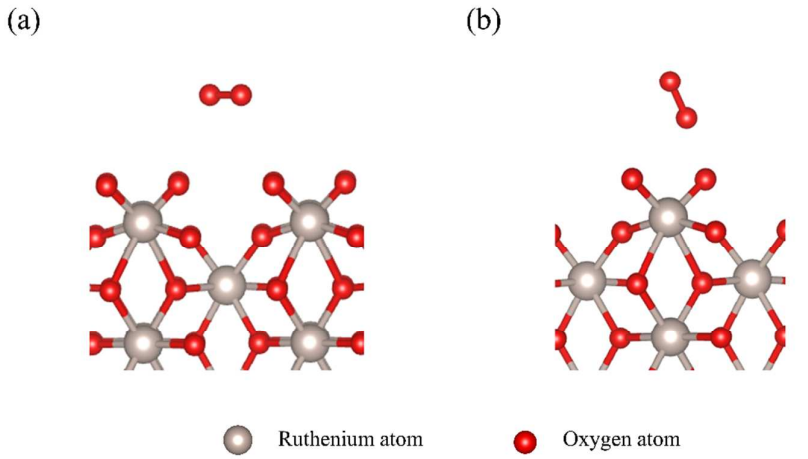

Fig. S4 Optimized geometry for oxygen molecular adsorbed onto rutile RuO_2 {001} surface. Two initial geometries were considered (a and b). The oxygen-oxygen bond lengths for both cases are 1.21Å (The bond length for free oxygen molecular is 1.21 Å).

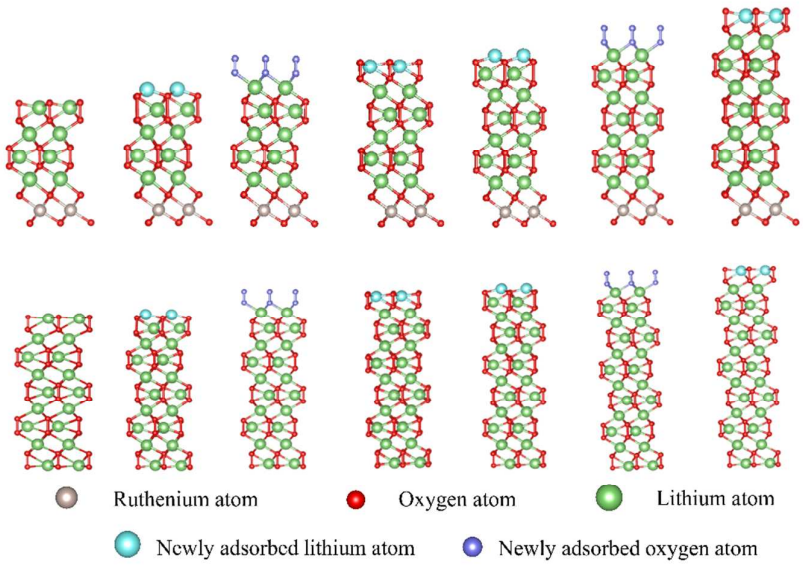

Fig. S5 Optimized geometry of discharge process happened on Li_2O_2 {0001} surface with and without RuO_2 monolayer.

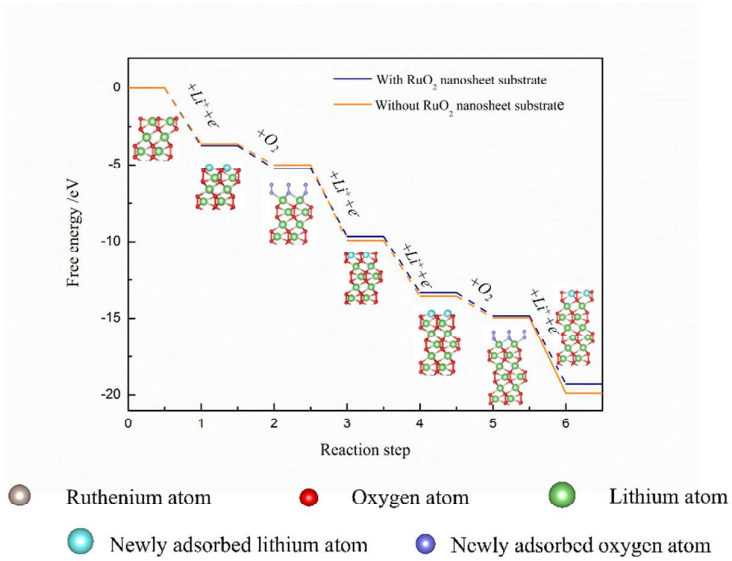

Fig. S6 Energy profiles for the discharge process happened on the Li_2O_2 {0001} surface with and without RuO_2 monolayer

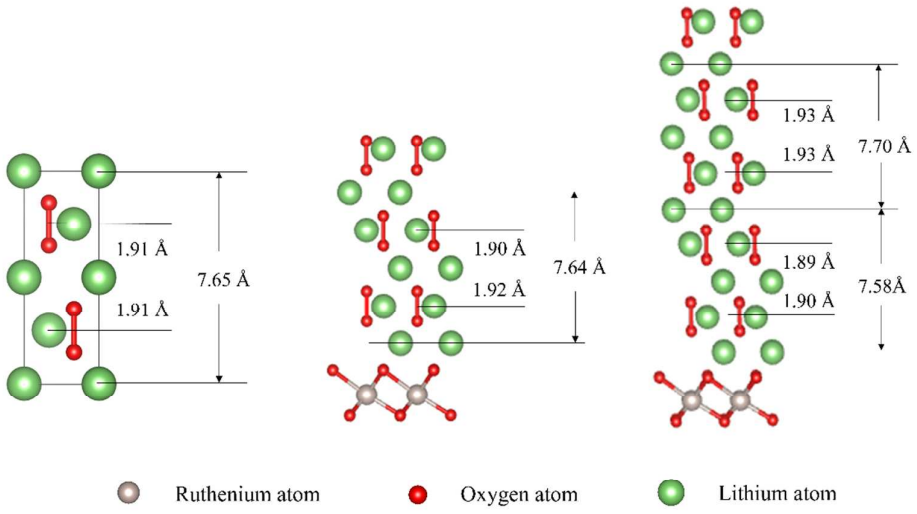

Fig. S7 Optimized lattice parameters of Li_2O_2 before and after adsorption onto RuO_2 monolayer.

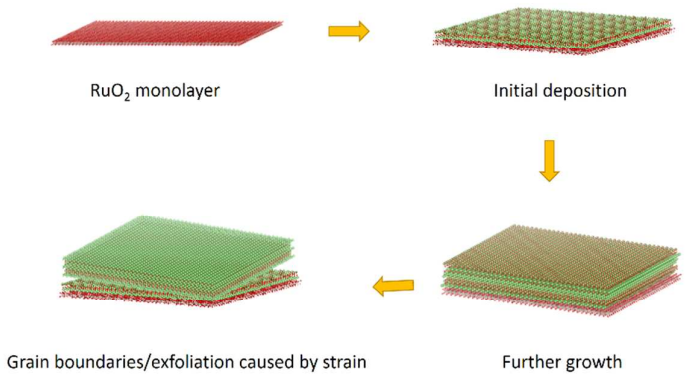

Fig. S8 Illustration for proposed formation mechanism for the assembled thin disc morphology of Li_2O_2

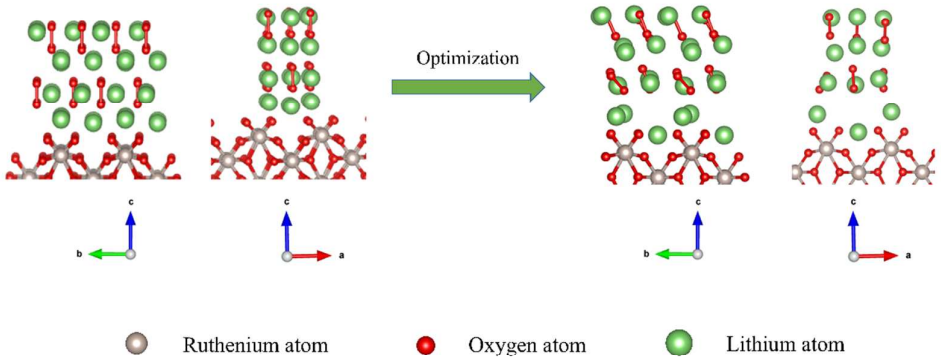

Fig. S9 The geometries of the interfacial model of rutile RuO_2 {001} surface and Li_2O_2 {0001} surface before and after optimization. The white, red and green balls correspond to ruthenium, oxygen and lithium atoms respectively.