Supporting Information

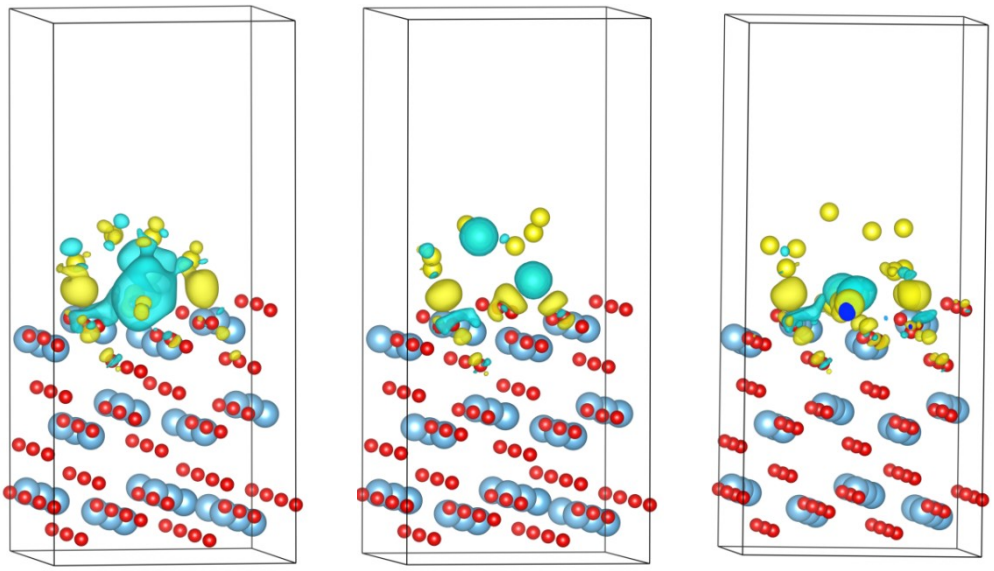
Adsorption of lithium polysulfides on an anatase (101) and an α-Al_2O_3(0001) surface under external electric field with first principles calculations

Table S1 Adsorption energies (eV) (with vdW) of the Li_2S_8 at other 10 different positions on an anatase (101) (E_{ad101}) surface.

Position	1	2	3	4	5	6	7	8	9	10	**Manuscript**
E_{ad101} (eV)	−2.45	−2.45	−3.78	−1.77	−2.45	−2.72	−2.72	−3.26	−2.25	−3.82	−3.84

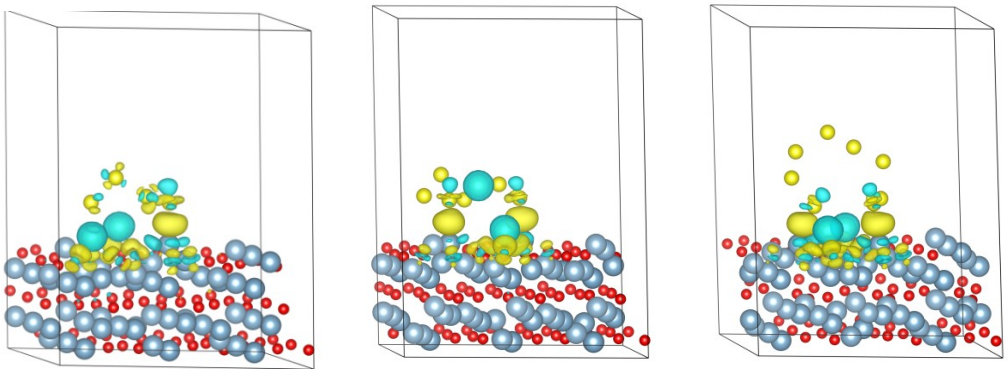
Table S2 Adsorption energies (eV) (without vdW) of the Li_2S_8 at 10 other different positions on an α-Al_2O_3 (0001) (E_{ad0001}) surface.

Position	1	2	3	4	5	6	7	8	9	10	**Manuscript**
E_{ad0001} (eV)	−2.96	−2.73	−1.99	−3.73	−3.75	−3.10	−2.64	−1.99	−2.70	−3.72	−4.14



(a) (b) (c)

Fig. S1 Charge density difference plot of (a) Li_2S_4, (b) Li_2S_6, and (c) Li_2S_8 on an anatase (101) surface. Yellow isosurfaces represent the increase of the electron density and blue isosurfaces represent the decrease of electron density.



(a) (b) (c)

Fig. S2 Charge density difference plot of (a) Li_2S_4, (b) Li_2S_6, and (c) Li_2S_8 on an α-Al_2O_3 (0001) surface. Yellow isosurfaces represent the increase in electron density and blue isosurfaces represent the decrease in electron density.

The charge density difference plot is obtained by subtracting the sum of the charge density of the adsorbed molecule and the slab from the charge density of the adsorbed system. The charge density of the molecule and the slab is obtained from the respective geometries in the optimized adsorption system (with vdW). The calculated charge density difference map has been plotted with isosurface value of 0.005 e/Å^3

and is shown in Fig. S1 and Fig. S2. In these plots, the yellow and blue isosurfaces indicate the gain and loss of electron density, respectively.

In Fig. S1 (a), the yellow isosurface is localized on the Ti atoms of anatase (101) surface and the blue isosurface is localized on the S atoms of Li_2S_4, indicating the charge transfer from the S atoms of Li_2S_4 to the Ti atoms of anatase (101) surface. Similarly, in the later cases the charge is transferred from the Li_2S_X to the anatase (101) surface (Fig. S1 (b, c)).

In Fig. S2 (a), the yellow isosurface is localized on the O atoms of the α-Al_2O_3 (0001) and the blue isosurface is localized on the Li atoms of Li_2S_4, indicating the charge transfer from the Li atoms of Li_2S_4 to the O atoms of the α-Al_2O_3 (0001). Similarly, in the later cases the charge is transferred from the Li_2S_X to the α-Al_2O_3 (0001) surface (Fig. S2 (b, c)).