Electronic Supplementary Information for

"*Mechanistic Insight into the Self-healing Capability of Solid-State Lithium Batteries: Role of the PEO-TiO_2 Interface*"

Federico Piciacchia[1], Sergio Tosoni[1*], Livia Giordano[1]

1 *Department of Materials Science, University of Milano-Bicocca, via Roberto Cozzi 55, Milan, Italy*

TabS1 : E_{vac}: O-vacancy formation energy; E_{ads}: adsorption energy of Li. The oxygen vacancy is located surface two-coordinate oxygen highlighted in FigS1;

U=4	E_{vac} (eV)	E_{ads}Li (eV)
2 layer	4.32	-1.14
3 layer	4.24	-1.67
4 layer	4.16	-1.71
U=3	E_{vac} (eV)	E_{ads}Li (eV)
2 layer	4.62	-1.65
3 layer	4.57	-1.77
4 layer	4.50	-1.84

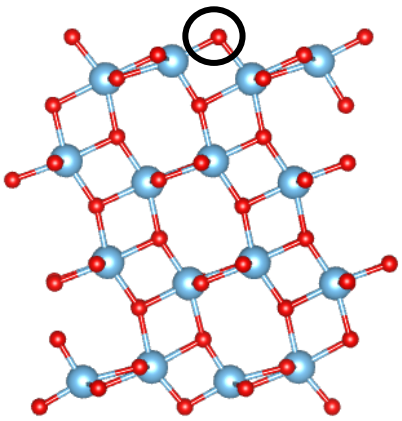

Fig. S1. Site of the surface oxygen vacancy.

At U=3 eV, as adopted in the present work, the adsorption energy of a Li atom, and the formation energy of an oxygen vacancy, (Table 1) display only a moderate dependency from the slab thickness. A similar statement holds true also for the band gap, Table S2. At U= 4 eV, the variations are more relevant.

* sergio.tosoni@unimib.it

Table S2 Energy gap calculated for 4 and 2 layers:

E_g (eV)	4 Layers	2 Layers
U=4	2.77	2.70
U=3	2.63	2.55

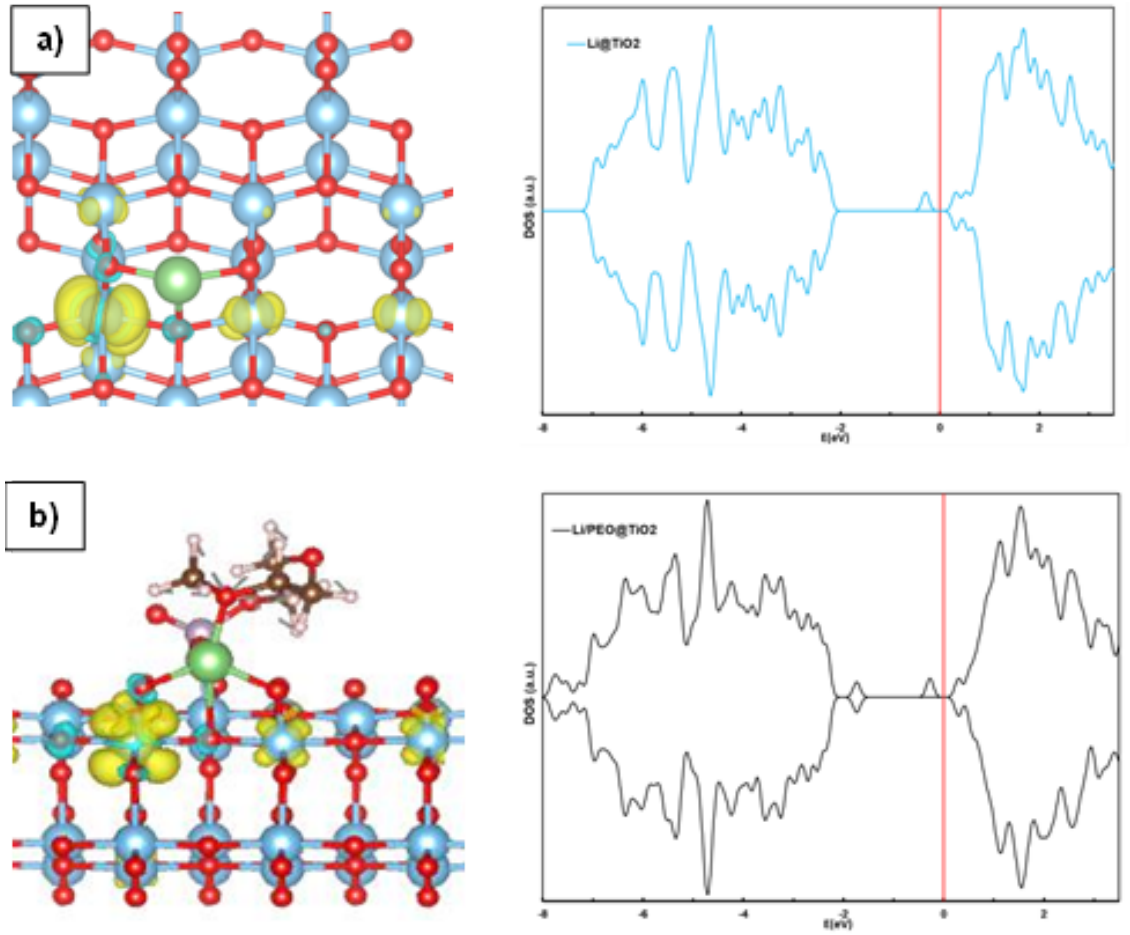

Fig.S2: a) Li@TiO_2 spin density (left) and total DOS (right); b) Li/PEO@TiO_2 spin density (left) and total DOS (right).