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

Supplementary Information
Catalytic properties of α-MnO_2 for Li-air battery cathodes: a density functional investigation

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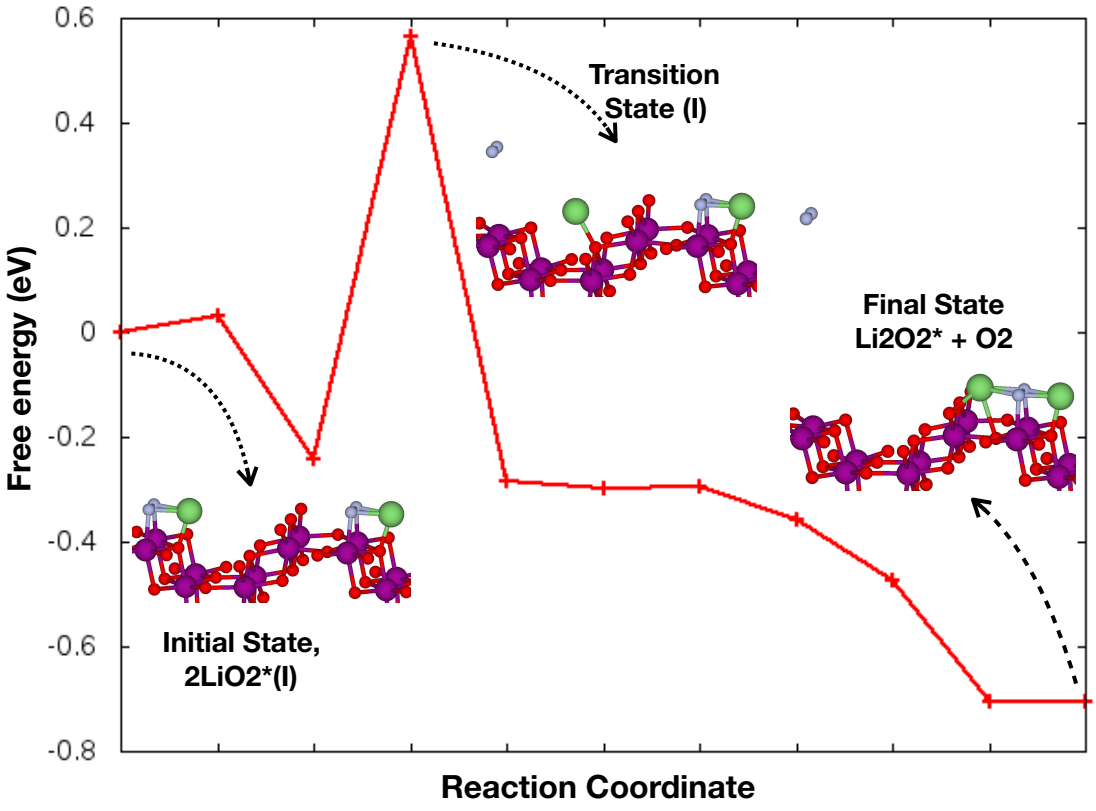

Figure S1: Free energies along the minimum energy path for the disproportionation reaction $2LiO_2$*(I) $\rightarrow$ Li_2O_2* + O_2 along path 1. Correction to the GGA energy of an isolated O_2 has been applied to all images except the first two in which O_2 is adsorbed on the surface. For the same reason, to calculate free energies, ZPE$-TS$ of the isolated O_2 molecule has been added to the energies of all the images except the first two.

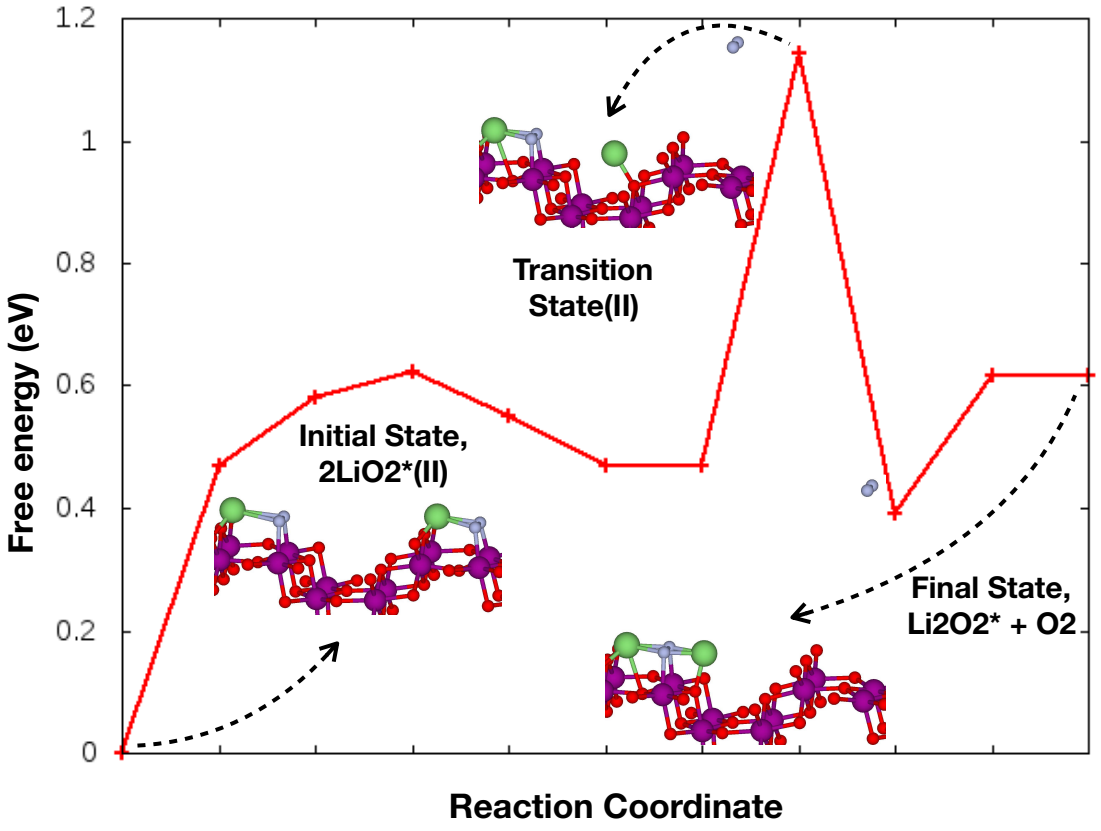

Figure S2: Free energies along the MEP of the disproportionation reaction $2LiO_2$*(II)→Li_2O_2* + O_2 along path 2. Same procedure as in case of path 1 has been used.