Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Phosphorene oxides as promising cathode materials for sealed non-aqueous Li-oxygen battery

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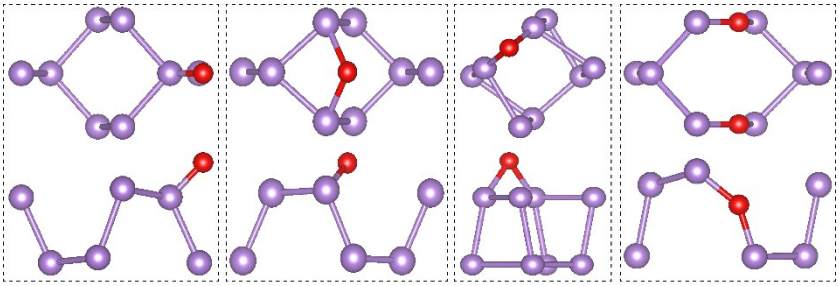

Fig.S1 Optimized stable structures of one O atom adsorbed on the surface of phosphorene. (a) O atom on top of P atom. (b) O above the center of the hexagonal ring. (c) O atom above the zigzag bridge of P-P bond. (d) O atom above the armchair bridge of P-P bond. The values below are the relative total energies of each structure with respect to the most stable one, which is set to 0 in (a).

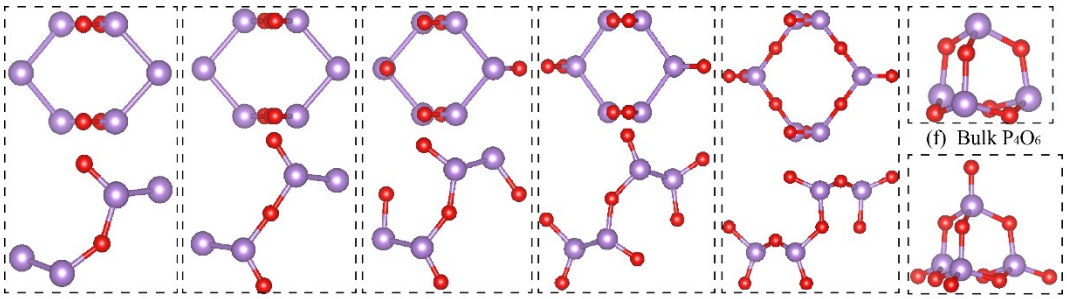

Fig.S2 Most stable structures of 2D-inter (a) P_4O_2, (b) P_4O_3, (c) P_4O_4, (d) P_4O_6, (e) P_4O_{10}, bulk (f) P_4O_6 and (g) P_4O_{10}.

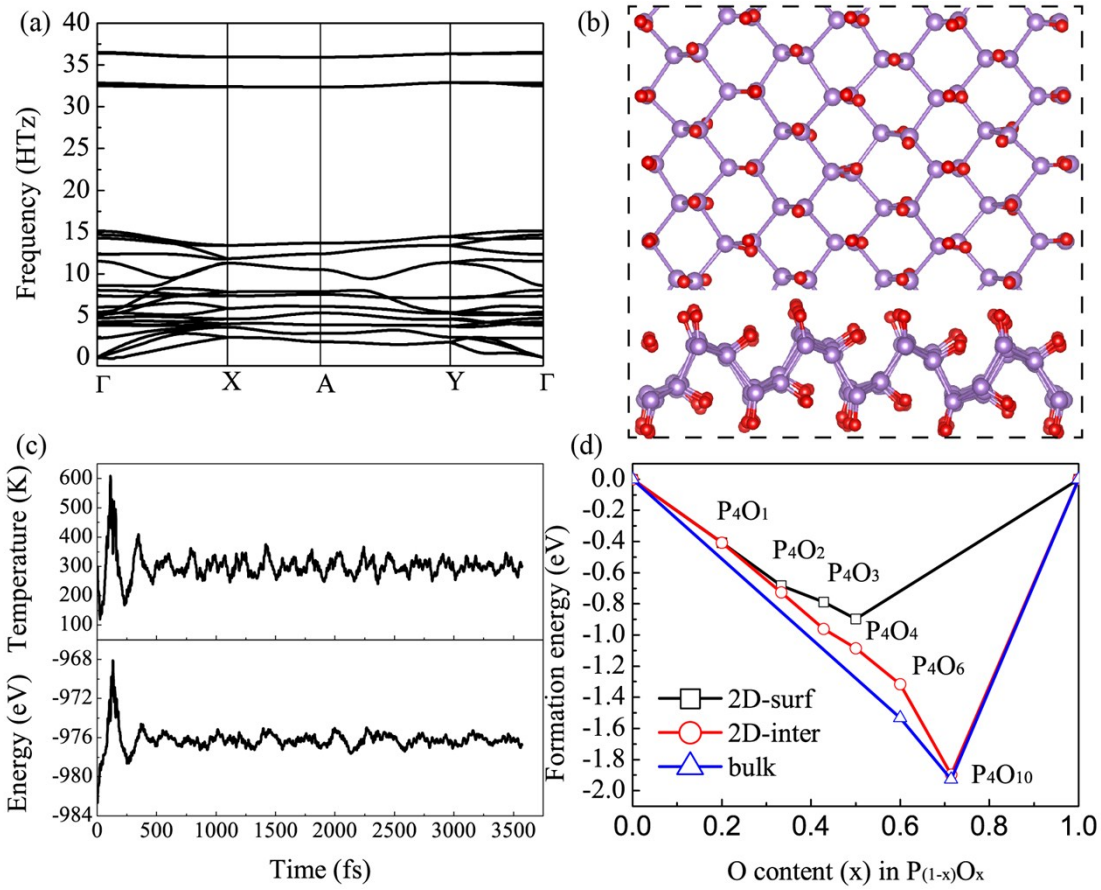

Fig.S3 (a) Phonon band dispersion of P_4O_4. (b) Snapshots of the crystal structure of P_4O_4 at the end of MD simulations. (c) Temperature and total energy evolutions of P_4O_4 as function of simulation time. (d) Formation energy as a function of O content.

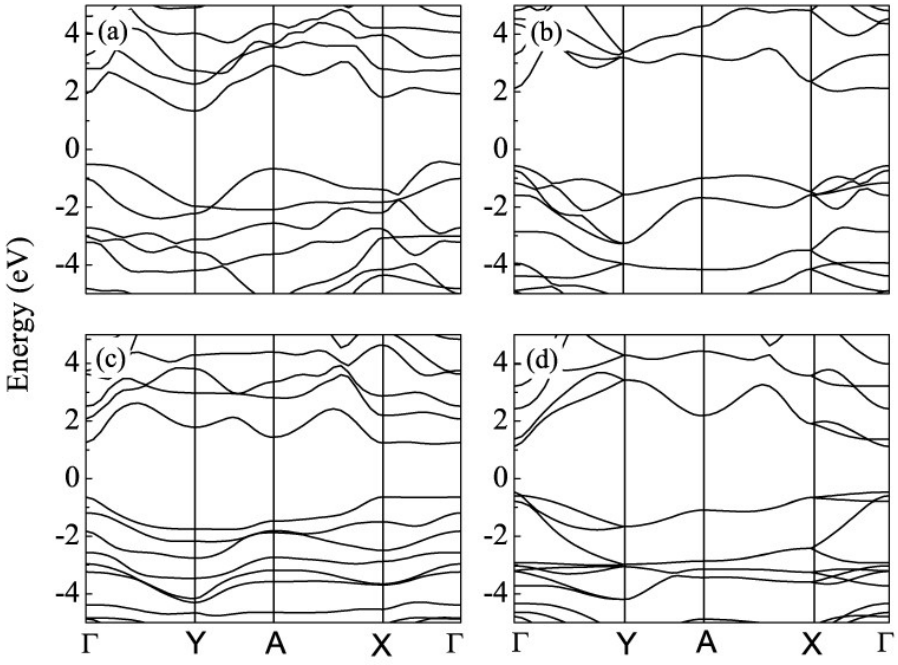

Fig.S4 Band structures of (a) P_4O_1, (b) P_4O_2, (c) P_4O_3 and (d) P_4O_4.

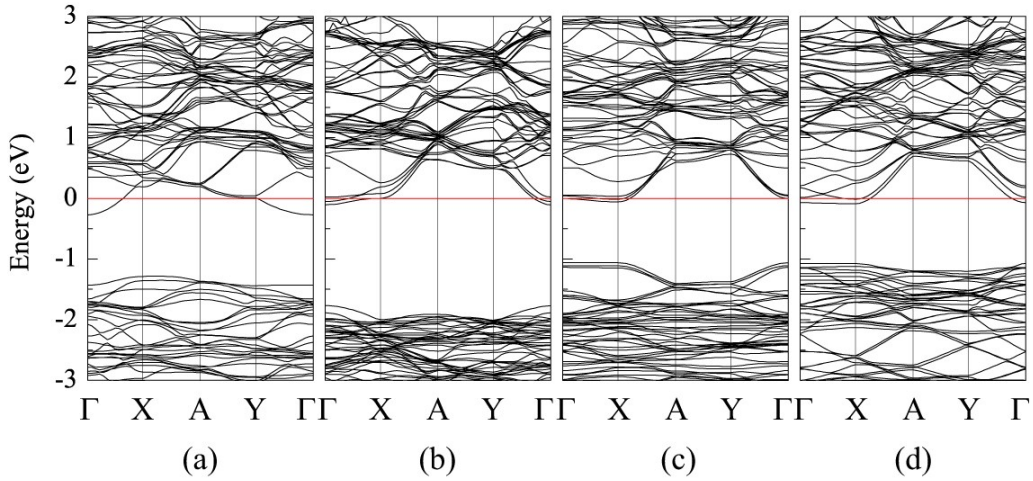

Fig.S5 Band structures of one Li adsorption on supercell containing 4×3 unit cells (a) P_4O_1, (b) P_4O_2, (c) P_4O_3 and (d) P_4O_4.

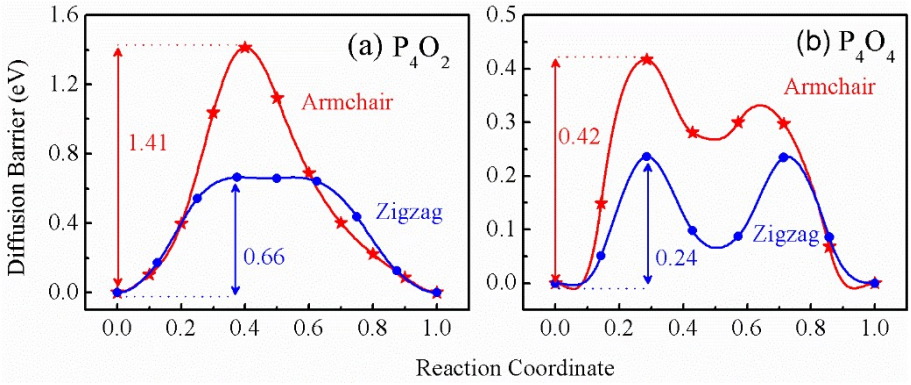

Fig.S6. Li diffusion barriers along the armchair and zigzag directions on (a) P_4O_2 and (d) P_4O_4.

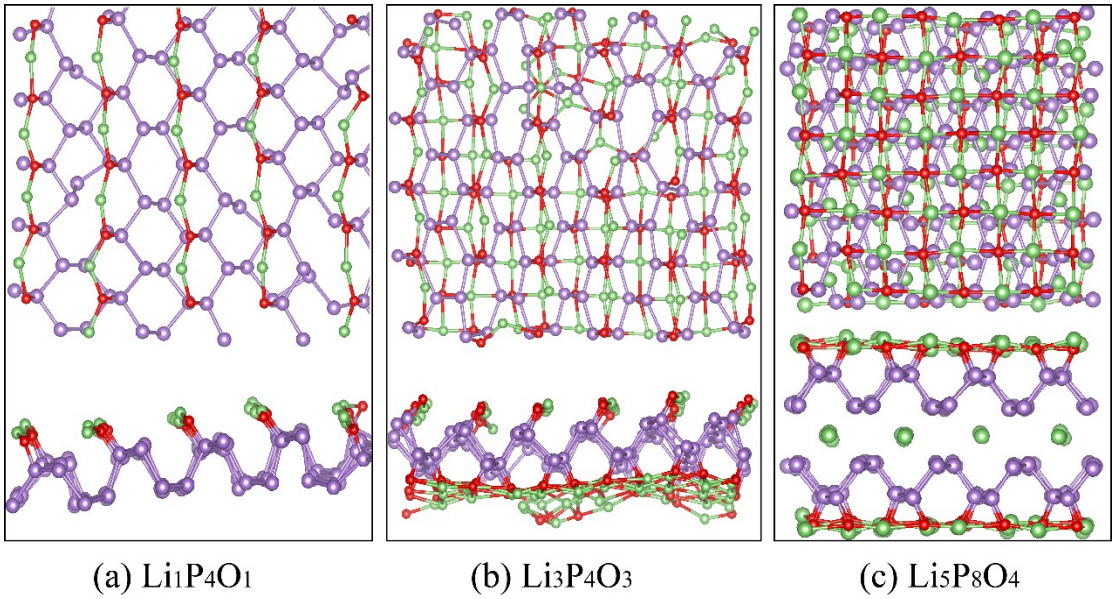

Fig.S7 Snapshots of the crystal structures of (a) $Li_1P_4O_1$, (b) $Li_3P_4O_3$ and (c) $Li_5P_8O_4$ at the end of the MD simulation.

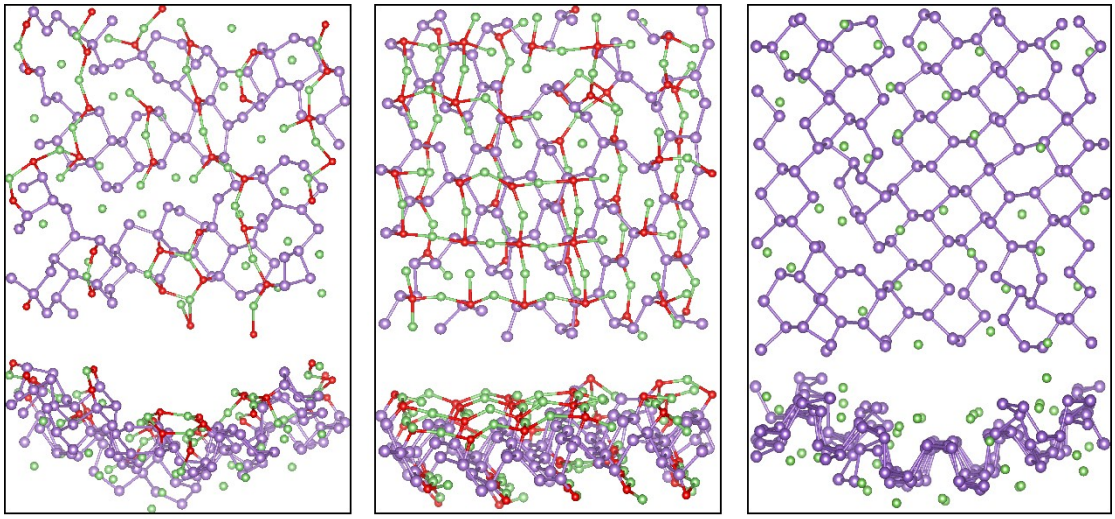

Fig.S8 Snapshots of the crystal structures of (a) $Li_2P_4O_1$, (b) $Li_3P_4O_2$ and (c) LiP_4 at the end of the MD simulation.

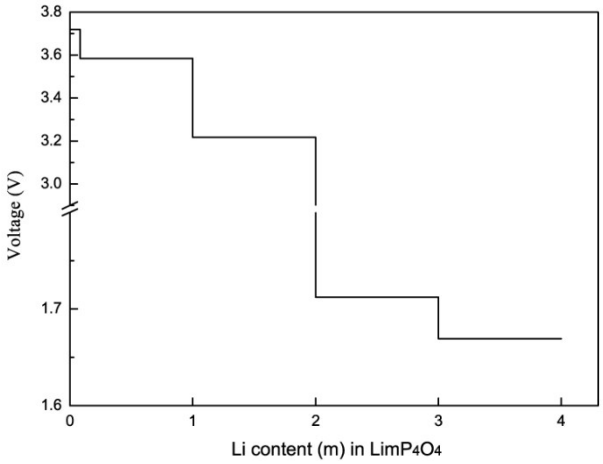

Fig.S9 Calculated voltage at every discharge stage of P_4O_4 cathode.