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Hydroxylated Carbon Black as Improved Deposition Support for Discharge Products in Lithium Air(Oxygen) Batteries

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The details of the binding energy calculations

The energy calculations were carried out using the Vienna ab initio simulation package(VASP).[1, 2] The projector augmented wave (PAW) method combined with a plane-wave basis set and a cut off energy of 400 eV was used to describe core and valence electrons.[3, 4] The Perdew-Burke-Ernzerhof (PBE) form of generalized gradient approximation (GGA)[5] was implemented in all calculations. Ground-state atomic geometries of the entire systems were obtained by minimizing the forces on each atom to below 0.05 eV/Å. The graphene substrate was modeled as a single sheet with (6 × 6) supercell (Fig. S2). A 15 Å thick vacuum layer was inserted between two sheets in the z direction. Brillouin k-point samplings for systems studied here were tested, a (3 × 3 × 1) k-point sampling scheme was applied to reach the accuracy of the calculations.

The adsorption energy ΔE_{ads} of the adsorbates on the surface is calculated through,

$$\Delta E_{ads}=E_{(substrate+adsorbate)}-E_{(substrate)}-E_{(adsorbate)}$$

Where $E_{(substrate\ +\ adsorbate)}$ is the total energy of the full system, and $E_{(substrate)}$ and $E_{(adsorbate)}$ are the total energies of its components.

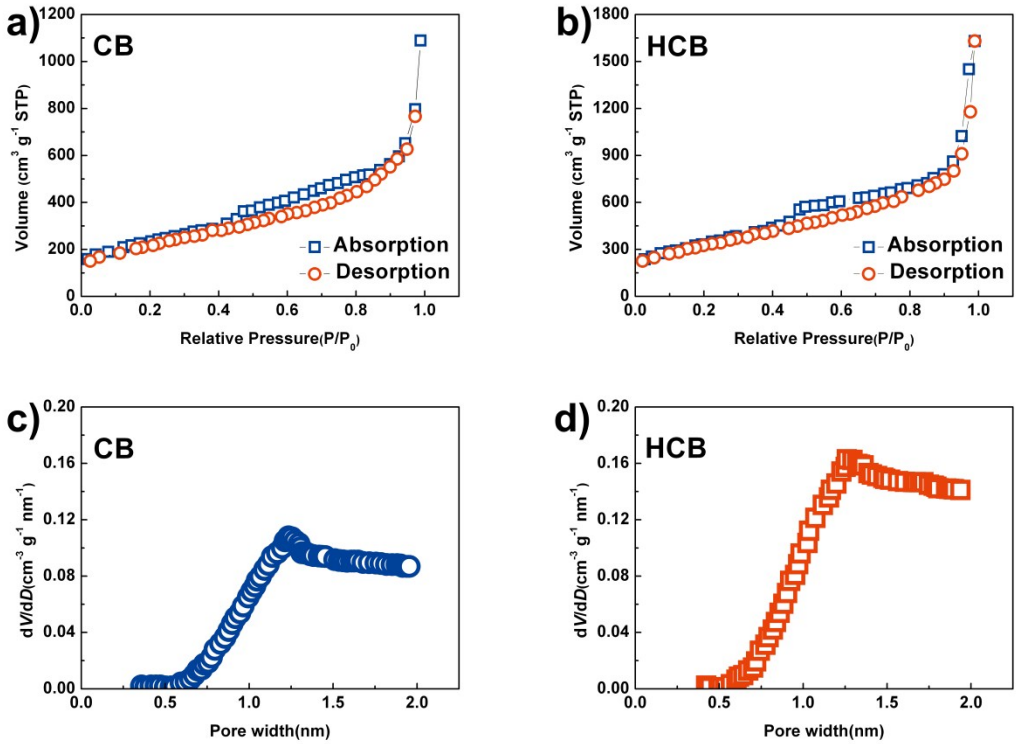

Fig. S1 N_2 absorption/desorption isotherms (a, b) and pore size distributions (c, d) of CB and HCB

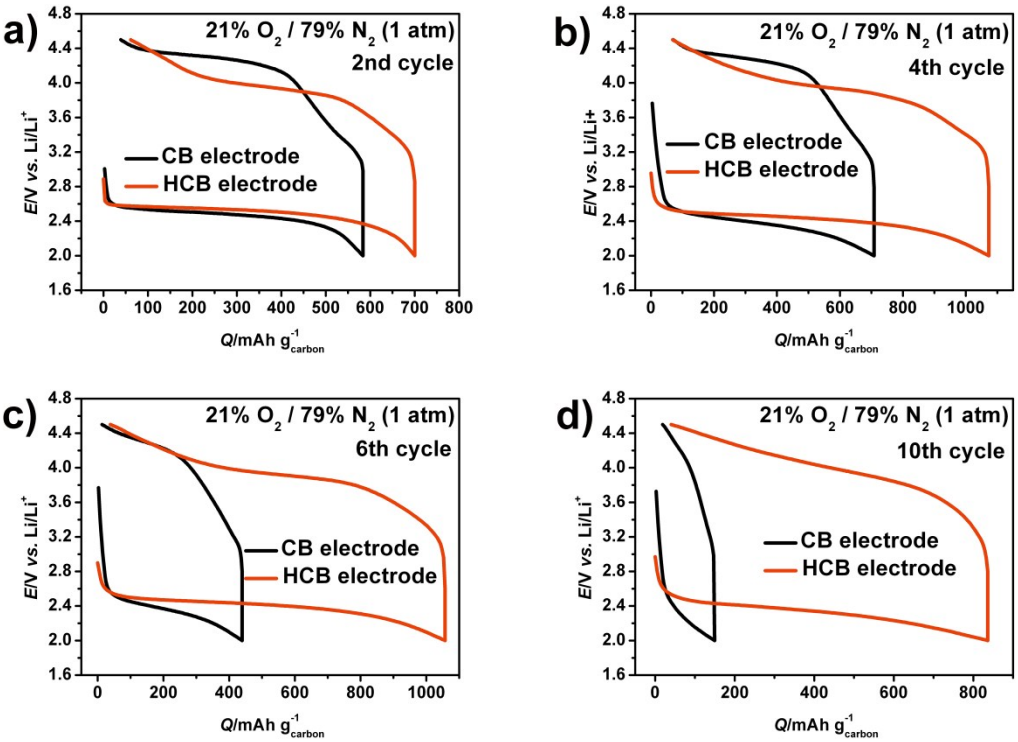

Fig. S2 Charge and discharge profiles of the CB and HCB electrodes during cycling. (a) 2nd. (b)4th. (c) 6th. (d) 10th.

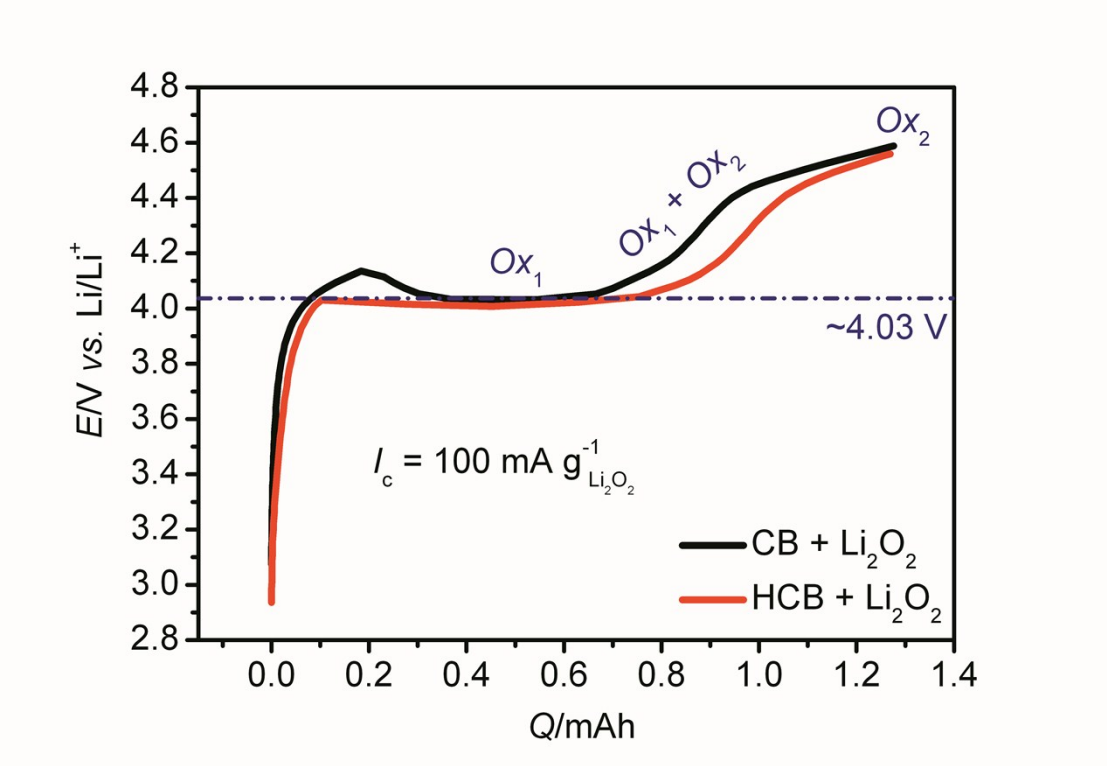

Fig. S3 Charge profiles of the CB+ commercial Li_2O_2 and HCB+ Li_2O_2 commercial cathodes

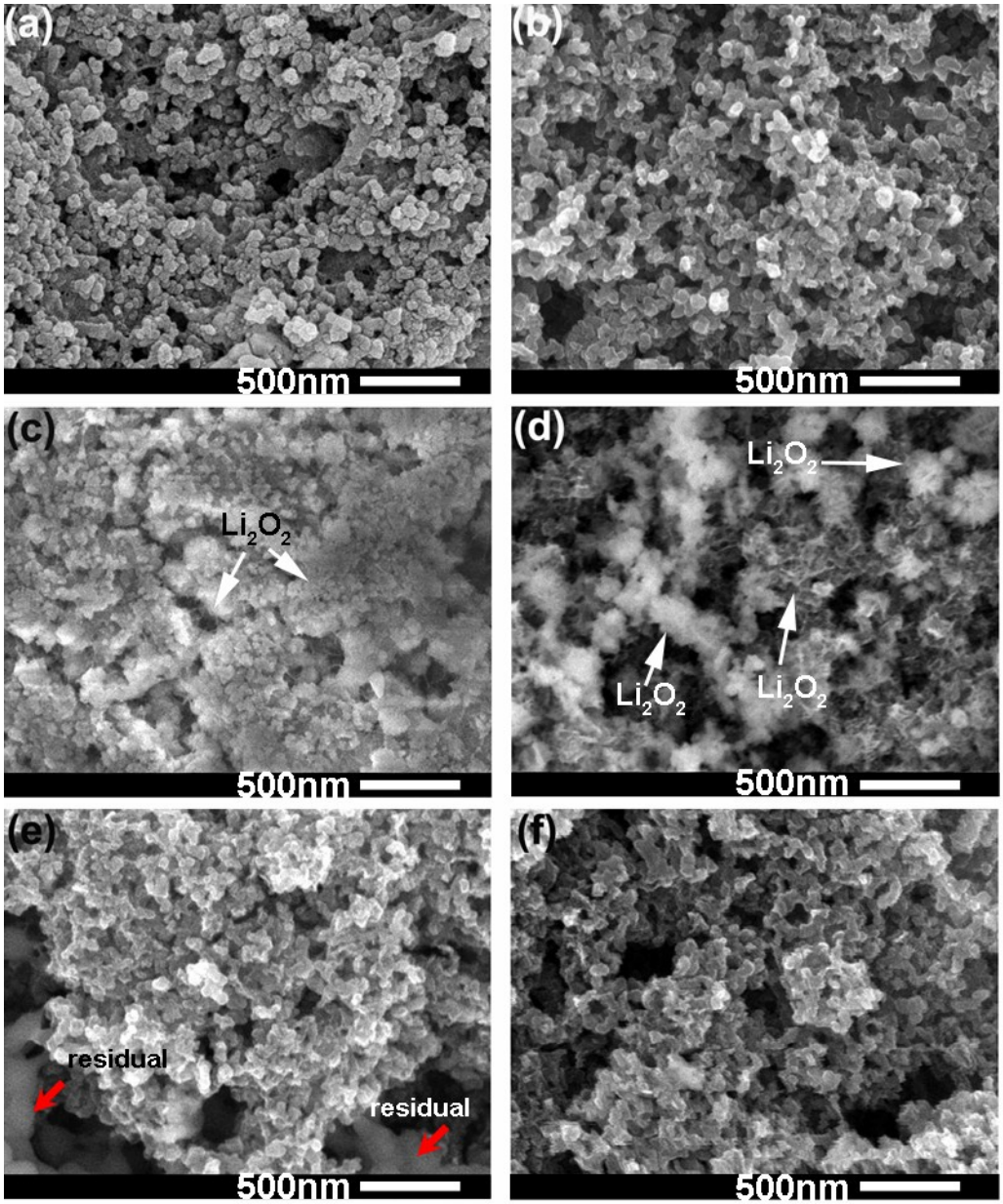

Fig. S4 FESEM images for CB (a, c, e) and HCB (b, d, f) electrodes, pristine (a, b), after 1st discharge (c, d), after 1st charge (e, f) respectively

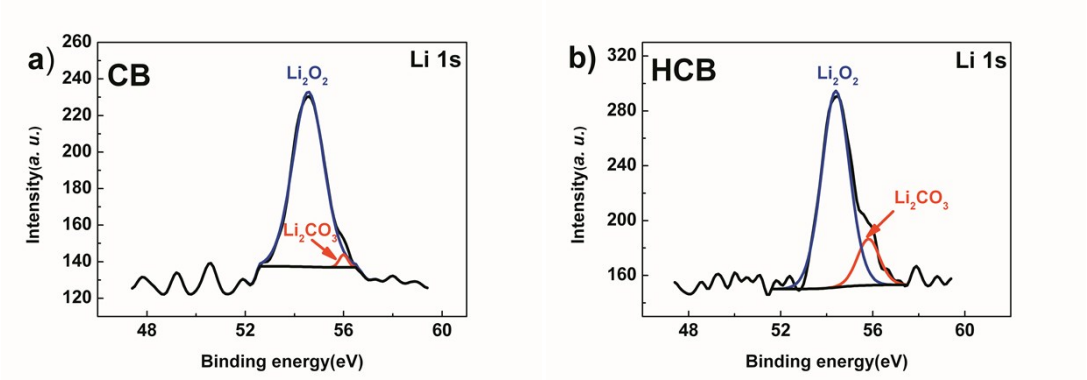

Fig. S5 XPS spectra (Li 1s) of the discharged CB (a) and HCB (b) cathodes

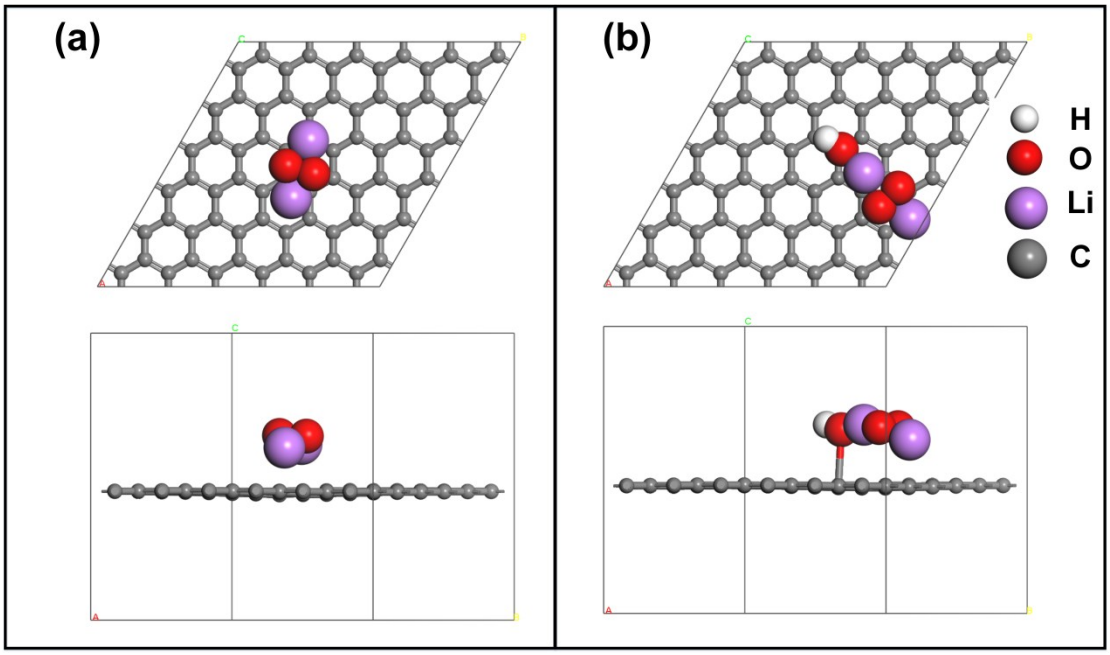

Fig. S6 Top and side views of optimized structure of Li_2O_2 on the common carbon black (a) and hydroxylated carbon black (b)

References

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