

Electronic Supplementary Information (ESI)

Double Perovskite Oxide $\text{Sr}_2\text{CrMoO}_{6-\delta}$ as an Efficient Electrocatalyst for Rechargeable Lithium Air Batteries

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Experimental Section

Material synthesis: The double perovskite oxide $\text{Sr}_2\text{CrMoO}_{6-\delta}$ (SCM) catalyst was synthesized by sol-gel and annealing method. Stoichiometric amounts of $\text{Sr}(\text{NO}_3)_2$ (4.23 g), $\text{Cr}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ (4.00 g) and $(\text{NH}_4)_6\text{Mo}_7\text{O}_{24} \cdot 4\text{H}_2\text{O}$ (1.77 g) were dissolved in deionized water (100 ml). Then, citric acid (12.61 g) and ethylene diamine tetraacetic acid (EDTA) (11.69 g) were added followed by vigorous stirring for 30 min at room temperature to form sols. The water in the sols was then evaporated at 65 °C for several hours to obtain the gels which were dried at 250 °C overnight followed by grinding into powders that were heat-treated, subsequently, at 800 °C in air for 6 h. Finally, the obtained powders were pressed into pellets at 300 MPa for 5 min and then annealed at 1200 °C for 24 h in 5 vol.% H_2/Ar mixed atmosphere to get the SCM catalyst.

Characterization: X-ray diffraction (XRD) pattern of the as-prepared double perovskite oxide $\text{Sr}_2\text{CrMoO}_{6-\delta}$ was collected with Rigaku D/max-2200/PC X-ray powder diffractometer. Morphology of the as-prepared SCM catalyst was acquired on FEI Sirion 200 scanning electron microscope (SEM) and JEM-2010HT transmission electron microscopy (TEM). The N_2 adsorption-desorption isotherm of the as-

prepared SCM catalyst was measured using Micromeritics ASAP 2010 M+C instrument at 77K and the specific surface area was calculated using the Brunauer-Emmett-Telley (BET) method. The XRD patterns of both the SCM based and pure Super P electrodes at various states were collected with Bruker D8 Advanced X-Ray Diffractometer, and the morphologies of the electrodes with/without SCM as catalyst were identified by a FEI Phenom G2 Pro X scanning electron microscope.

Cell assembly: The air electrode was prepared by a spray method as reported in our previous works¹ employing nickel foam (thickness: 1.7 mm; area density: 420 g m⁻²; porosity: 110 ppi; Heze Tianyu Technology Development Co., Ltd. China) as the substrate. The slurry composed of SCM catalyst, Super P (SCM Industrial Chemical Co., Ltd.) and polytetrafluoroethene (PTFE) in a weight ratio of 30:60:10 was obtained by uniformly dispersing the materials in ethanol. A lithium metal anode, a glass fiber separator, an as-prepared air electrode and an electrolyte of 0.1 M LiTFSI (lithium bis-(trifluoromethanesulfonyl)-imide) in TEGDME (tetraethylene glycol dimethyl ether) were employed to assemble the electrochemical battery in an argon-filled glove box with oxygen and water contents less than 0.1 ppm.

For comparison, the pure carbon electrode without catalyst was also prepared using 90 wt.% Super P and 10 wt.% PTFE to assemble the Li-air batteries with the same procedures as described above.

Electrochemical Measurements: The electrochemical performance of the batteries was evaluated in a 1 atm O₂ atmosphere using a LAND CT2001A battery testing system at room temperature. Before the galvanostatic discharge/charge measurements, the batteries were placed in flowing pure oxygen for 1 h and then transferred into the oxygen filled glass container for 6 h. The specific capacity and current density were calculated based on the amount of carbon material in the electrode. The cyclic voltammograms were recorded within a potential range of 2.0-4.5 V under O₂ atmosphere and within 1.8-5.0 V under Ar atmosphere for both SCM based and pure Super P electrodes with a potential scanning

rate of 0.5 mV s^{-1} at room temperature controlled by a CHI 750a. The electrochemical impedance spectroscopy (EIS) was measured in a frequency range from 1000 kHz to 10 mHz.

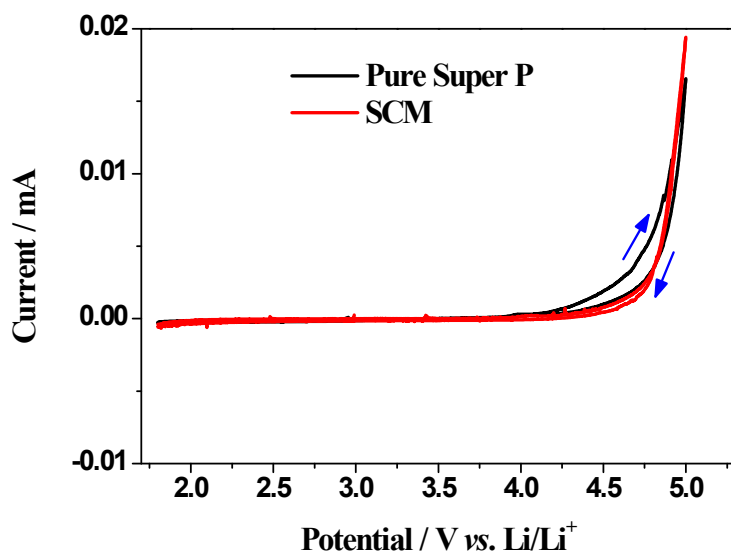


Fig. S1 Cyclic voltammograms of 0.1 M LiTFSI/TEGDME on SCM based electrode and pure Super P electrode under Ar atmosphere

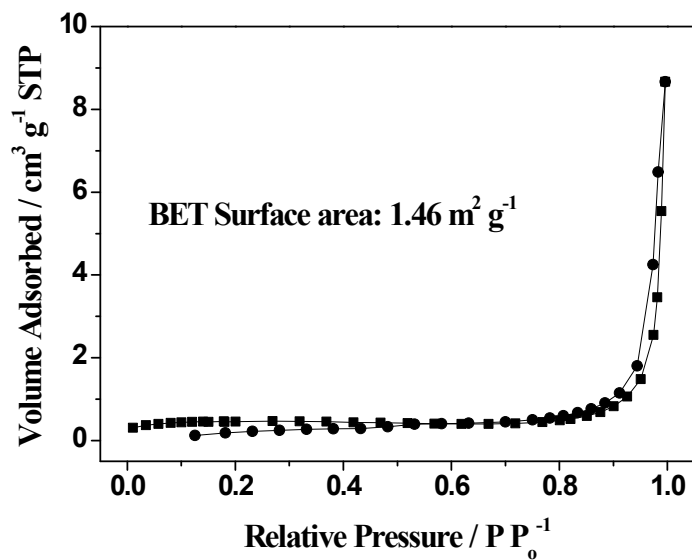


Fig. S2 N₂ adsorption-desorption isotherm of the double perovskite oxide SCM

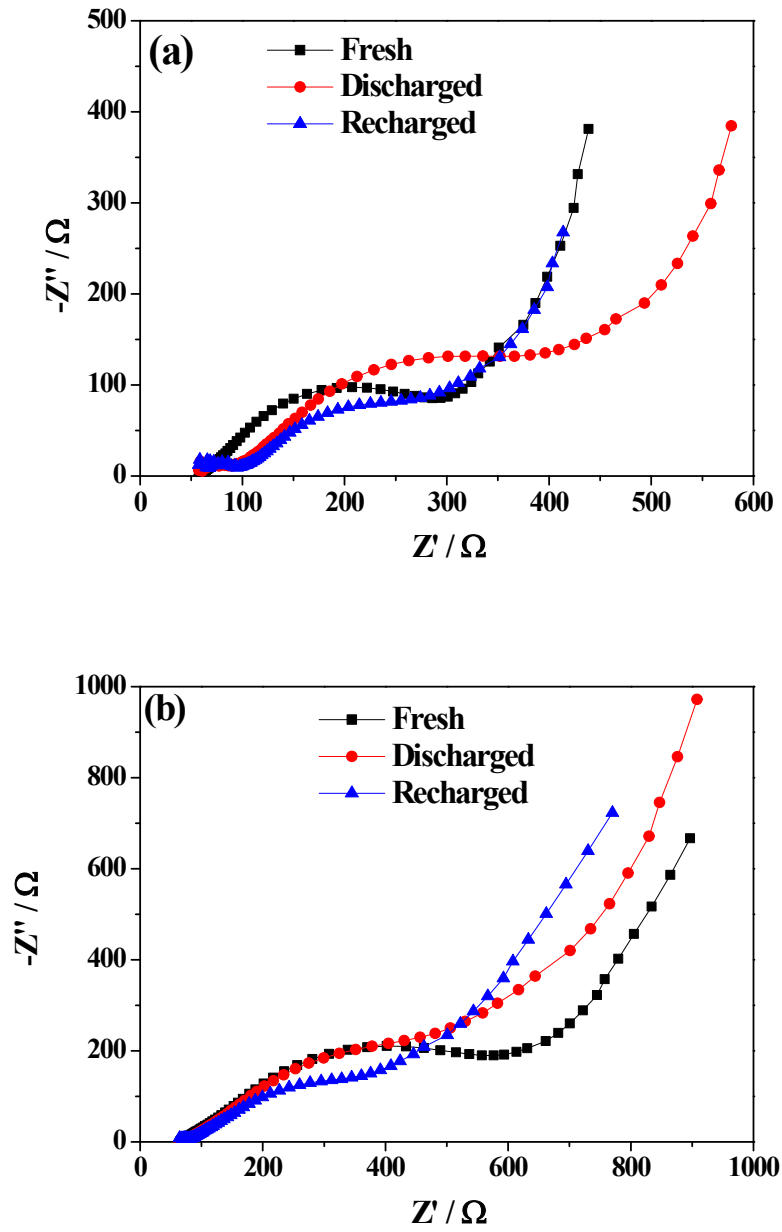


Fig. S3 Electrochemical impedance spectra of SCM based (a) and pure Super P (b) electrodes at various states

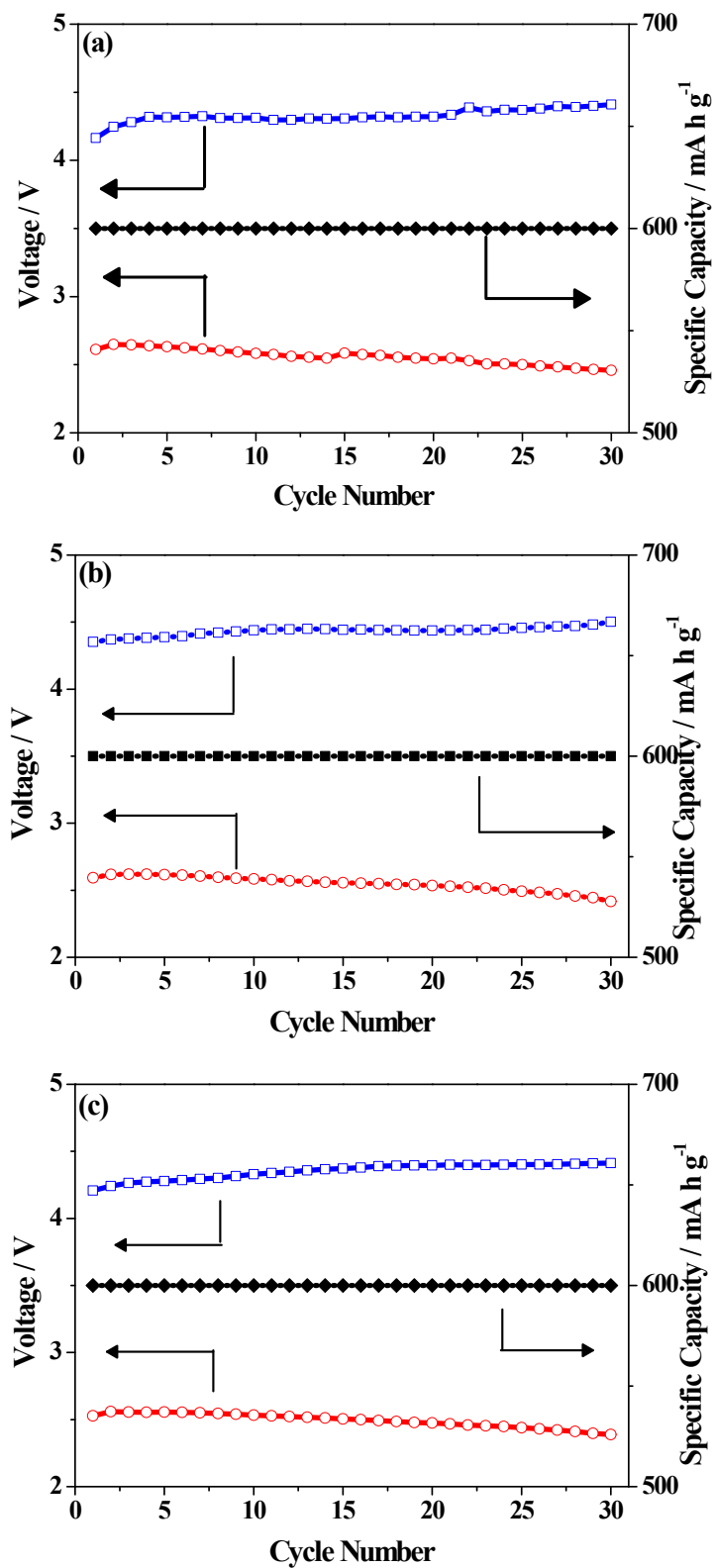


Fig. S4 Terminal discharge and charge voltages versus cycle numbers for the SCM based cathode at various current densities (75 (a), 150 (b) and 200 (c) mA g⁻¹)

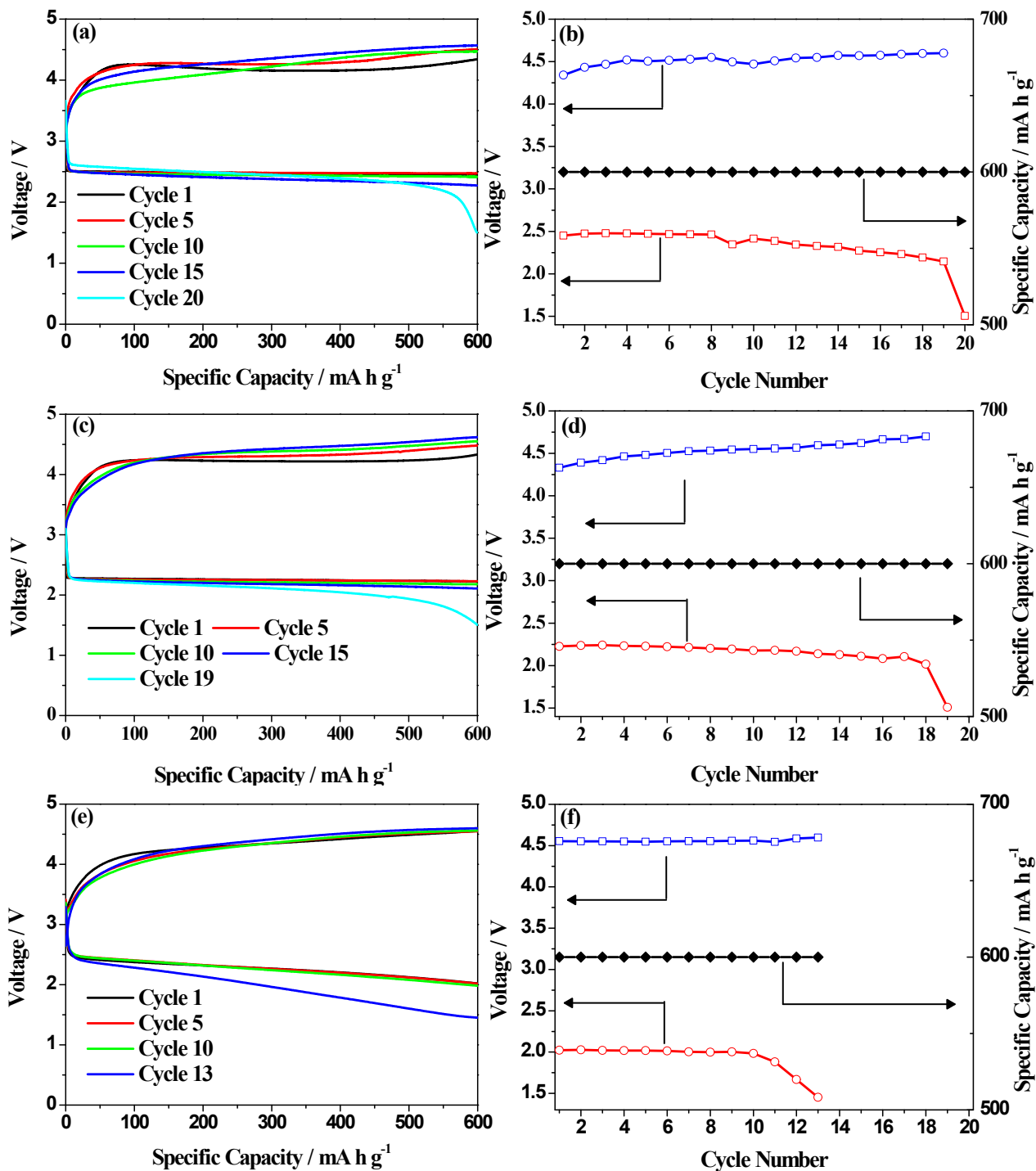


Fig. S5 Discharge-charge profiles and terminal voltages of the Li-air batteries with pure Super P cathode versus cycle numbers at various current densities (75 (a, b), 150 (c, d) and 200 (e, f) mA g⁻¹).

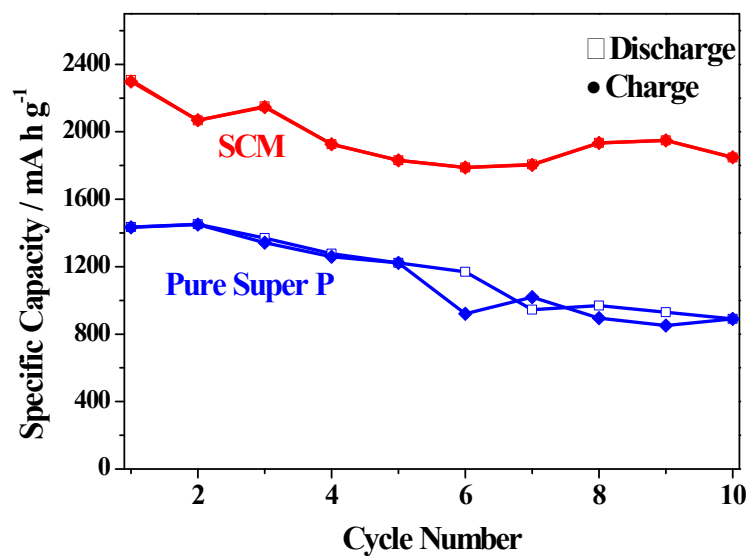


Fig. S6 Discharge/charge capacities versus cycle number for the SCM based and pure Super P cathodes at a current density of 75 mA g^{-1} .

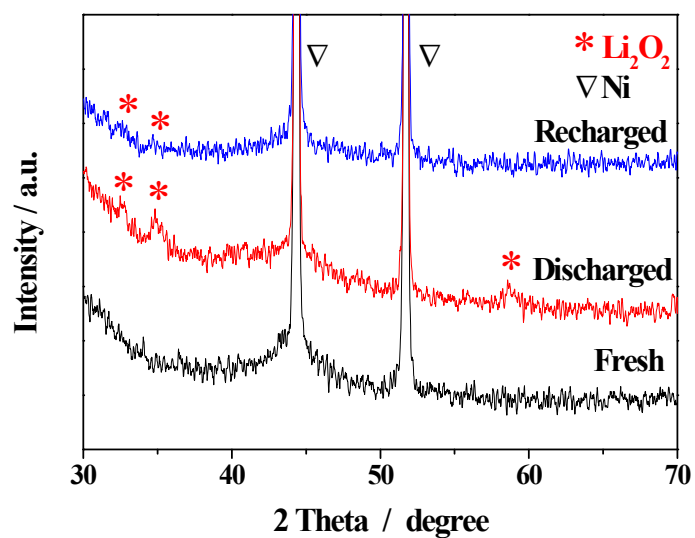


Fig. S7 XRD patterns of fresh, discharged and recharged pure Super P electrodes

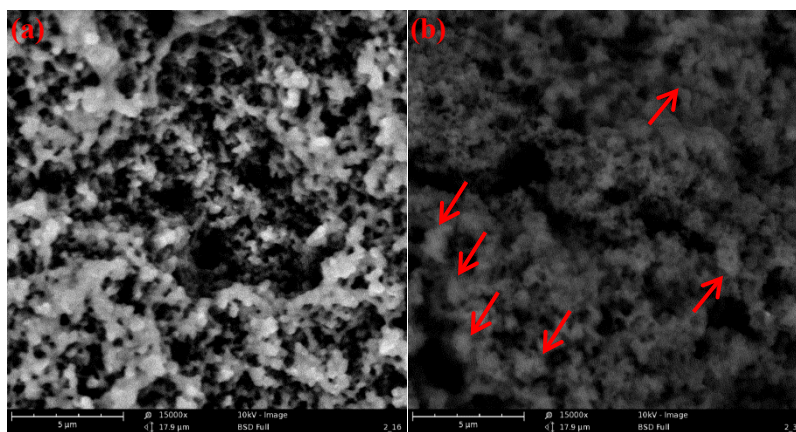


Fig. S8 SEM images of the pure Super P electrodes: discharged (a) and recharged (b).

References

- 1 Z. Ma, X. Yuan, H.-D. Sha, Z.-F. Ma and Q. Li, *Int. J. Hydrogen Energ.*, 2013, **38**, 11004.