Electronic Supporting Information (ESI)

MoS_2 nanosheets decorated with gold nanoparticles for rechargeable Li-O_2 batteries

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1.1 Reagents and materials

Ammonium tetrathiomolybdate ($(NH_4)_2MoS_4$) and chloroauric acid ($HAuCl_4 \cdot 3H_2O$, ≥49.0% Au basis) were purchased from J&K Scientific Ltd. (Beijing, China). Lithium trifluoromethanesulfonate (99.9%), N-methyl-2-pyrrolidone (NMP, 99.5%), $LiCF_3SO_3$-TEGDME electrolyte, poly-vinylidenefluoride (PVDF), and ethanol were obtained from Sigma-Aldrich. Hydrazine ($N_2H_4 \bullet H_2O$) was supplied by Beijing Chemicals Co., Ltd. (Beijing, China). All chemicals used in this work were of analytical reagent grade and obtained from commercial sources and directly used without additional purification. The water used was purified through a Millipore system (~18.2 MΩ·cm). Carbon-coated Cu grids for transmission electron microscopy (TEM) characterization were purchased from Plano GmbH (Wetzlar, Germany).

1.2 Experimental techniques

TEM and HRTEM characterizations were conducted on a JEM-2100F field emission transmission electron microscopy operated at 200 kV. The samples were prepared by dropping the MoS_2/AuNP nanohybrid aqueous solution onto the copper grid, and dried at room temperature. Scanning electron microscopy (SEM, JSM-6700F, JEOL, Japan), X-ray diffraction (XRD, Rigaku D/max-2500 VB+/PC), X-ray photoelectron spectroscopy (XPS, ThermoVG ESCALAB 250), and Raman spectroscopy (LabRAM HORIBA JY, Edison, NJ) were used to compare the structures and morphologies of MoS_2 nanoflowers with MoS_2/AuNP nanohybrids. The specific surface area and pore size characterizations were performed by 3H-2000PS1 static volume method with specific surface & pore analysis instrument (BeiShiDe, Beijing).

1.3 Preparation of MoS_2 nanoflowers and MoS_2/AuNP nanohybrids

For the preparation of MoS_2 nanoflowers, 22 mg of $(NH_4)_2MoS_4$ was added to 20 mL of DI water and sonicated for 10 min to achieve a clear and homogeneous solution. After that, 50 μL of hydrazine was added. The reaction solution was further sonicated for 30 min before transferred to a 50 mL Teflon-lined autoclave. It was heated in an oven at 200 ^oC for 10 h with no intentional

control of ramping or cooling rate. To prepare MoS_2/AuNP nanohybrids, 22 mg of $(NH_4)_2MoS_4$ and $HAuCl_4$ (100 μL, 507.83 mM) was mixed into 20 mL of DI water and sonicated for 10 min. After that, 100 μL of hydrazine was added. The reaction solution was further sonicated for 30 min before transferred to a 50 mL Teflon-lined autoclave. It was heated in an oven at 200 °C for 10 h without intentional control of ramping or cooling rate. Product was both centrifuged at 4500 rpm for 10 min with DI water and ethanol, and each washing step was repeated for at least 3 times. Finally, product was re-dispersed in 3 ml of DI water and frozen drying for several days. The typical yield was ~90%. Based on the XPS spectra and EDX analysis of MoS_2/AuNP nanohybrids, we calculated the weight ratios of MoS_2 and AuNPs, which were 81.8 and 18.2 wt%, respectively.

1.4 Characterizations of MoS_2 nanoflowers and MoS_2/AuNP nanohybrids

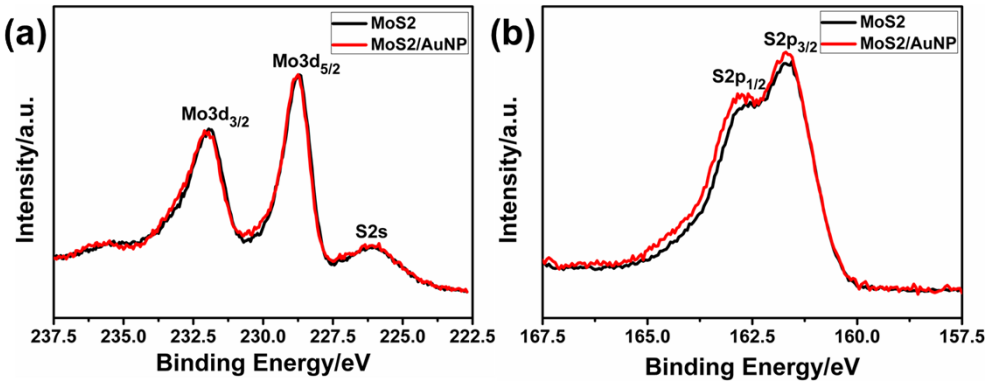

Fig. S1 XPS spectra for (a) Mo and (b) S binding energies of MoS_2 nanoflowers and MoS_2/AuNP nanohybrids.

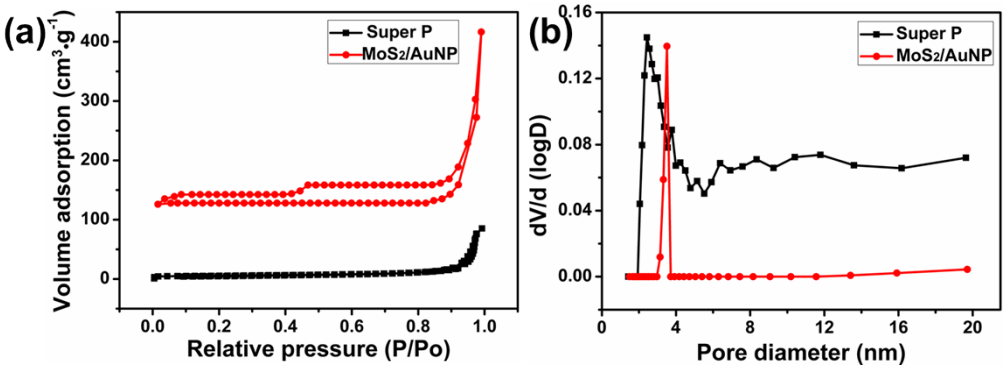

Fig. S2 (a) Nitrogen-adsorption-desorption isotherms, (b) pore-size distributions of Super P and MoS_2/AuNP nanohybrids.

1.5 Fabrication of Li-O_2 battery (half cells)

Electrochemical experiments were performed using Swagelok-type cells. Li-O_2 battery was fabricated using a lithium foil as the negative electrode, a 1.0 M solution of $LiCF_3SO_3$ in TEGDME as the electrolyte, and a pellet made of the MoS_2/AuNP nanohybrids, Super P and PVDF (binder, solvent: NMP) in a weight ratio of 2:6:2 as the positive electrode. The specific surface area of MoS_2/AuNP nanohybrids is 213.6 $m^2 \cdot g^{-1}$, while that of Super P is 62.0 $m^2 \cdot g^{-1}$. In addition, the average density of each cathode for parallel test is 0.5 $mg \cdot cm^{-2}$. Whatman glass fiber was used to separate the Li anode and the cathode. The battery cell was assembled in an argon-filled glove box with the H_2O and O_2 concentrations below 1.0 ppm. The electrochemical properties were studied with a multichannel battery-testing system (Arbin BT 2000). Galvanostatic charge-discharge cycling was performed over a voltage window of 2.0-4.5 V. The working electrode was measured at room temperature during the whole process. In order to avoid any negative effects of humidity and CO_2, the batteries were sealed except for the cathode exposed to 1 atm O_2 pressure. Cyclic voltammetry (CV) was performed by a potentiostat (IM6, Zahner elektrik) connected to a personal computer and controlled by the Thales software package.

1.6 Characterizations of Li-O_2 battery (half cells)

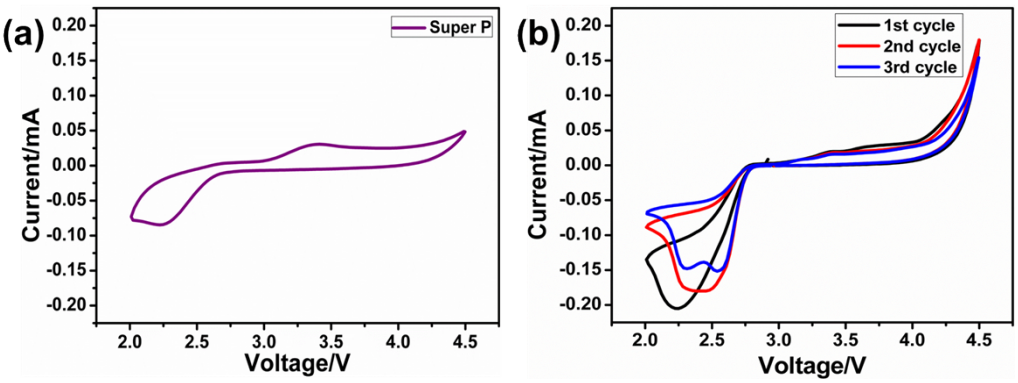

Fig. S3 CVs of (a) Super P and (b) MoS_2/AuNP nanohybrids with the first to three cycles at 0.1 $mV \cdot s^{-1}$ scan rate and voltage of 2.0 V to 4.5 V.

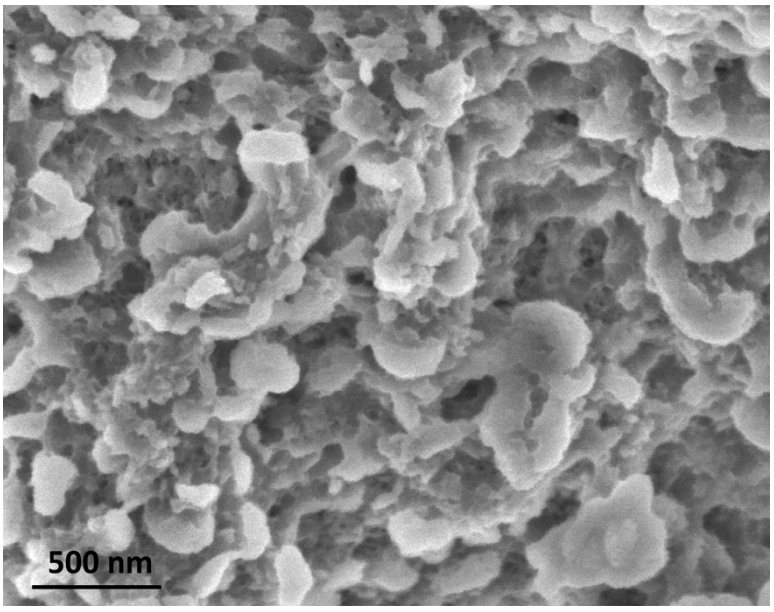

Fig. S4 SEM image of the electrode modified with MoS_2/AuNP nanohybrids after discharging.

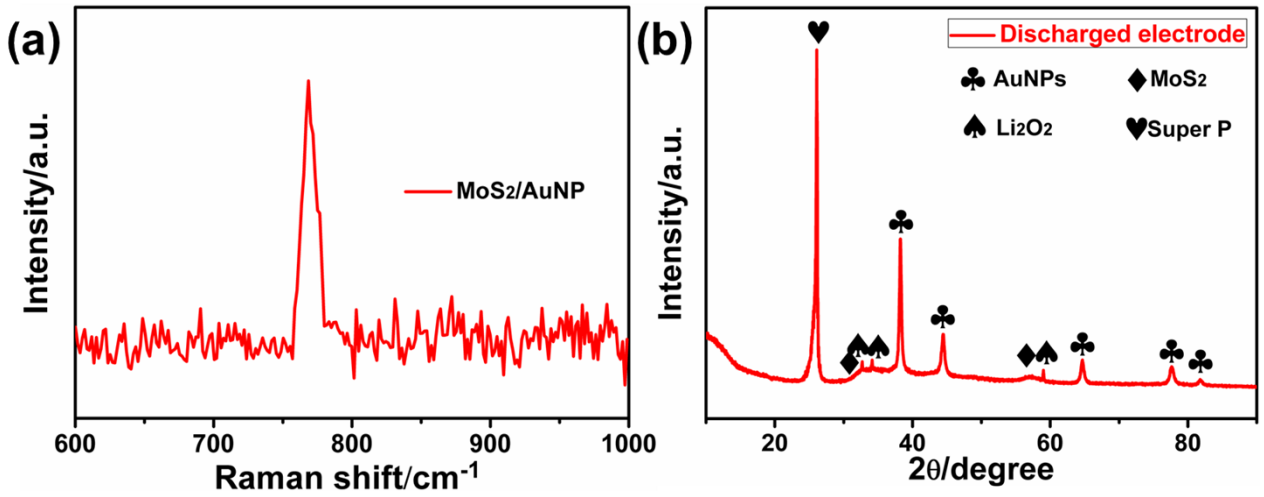

Fig. S5 (a) Raman spectrum and (b) XRD pattern of the discharge product on the electrode modified with MoS_2/AuNP nanohybrids.