Supplementary Information

A disc- like Mo- metal cluster compound, Co$_2$Mo$_3$O$_8$, as a high capacity anode for lithium ion batteries

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X-ray diffraction (XRD) analysis of Co$_2$Mo$_3$O$_8$ composite electrode heated at 300 °C, 12 h, Ar-atm.

Fig. S1 X-ray diffraction patterns of Co$_2$Mo$_3$O$_8$ composite electrode heated at 300 °C, 12 h, Ar-atm. Miller indices ($h$ $k$ $l$) are shown. The characteristic lines due to Cu are from the current collector. Co- impurity is from the material. The y- axis values are normalized for better comparison at various voltages.
Ex-situ XRD of Co$_2$Mo$_3$O$_8$ composite electrode during 1$^{st}$ cycle.

![X-ray diffraction patterns of Co$_2$Mo$_3$O$_8$ composite electrode.](image)

Fig. S2 X-ray diffraction patterns of Co$_2$Mo$_3$O$_8$ composite electrode. (a) Bare electrode. (b) 1$^{st}$ discharge; 1.0 V. (c) 1$^{st}$ discharge; 0.005 V. (d) 1$^{st}$ charge; 3.0 V. The characteristic lines due to Cu are from the current collector. Co- impurity is from the material. The y- axis values are normalized for better comparison at various voltages.
Ex-situ TEM of Co$_2$Mo$_3$O$_8$ composite electrode at 1$^{st}$ discharge to 0.005 V.

Fig. S3 Ex situ TEM for the cycled electrode (at 60 mA g$^{-1}$) of Co$_2$Mo$_3$O$_8$ during 1$^{st}$ discharge to 0.005 V. (a) TEM image and (b) SAED pattern. Scale bars are shown.

**Sample preparation:**

**Ex-situ XRD:** The composite electrode was discharged and charged during 1$^{st}$ cycle to selected voltages at 60 mA g$^{-1}$. The cells were opened inside glove box and the electrodes were collected. The electrode were washed with DMC for 2-3 times and dried. The electrodes were placed on the XRD sample holder and sealed by para film to avoid oxidation. The XRD measurement was carried out using Philips X’PERT MPD diffractometer equipped with Cu K$_\alpha$ radiation.

**Ex-situ TEM:** Similar procedure was followed as discussed in the ex-situ XRD sample preparation. But, after drying the electrode materials were scratched from the current collector and dispersed in absolute ethanol by using ultra-sonication. The suspension was deposited on a holey carbon grid. The TEM measurement was carried out as discussed in the experimental section in the manuscript.