Supplementary Information

A disc- like Mo- metal cluster compound, $Co_2Mo_3O_8$, as a high capacity anode for lithium ion batteries

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X-ray diffraction (XRD) analysis of $Co_2Mo_3O_8$ composite electrode heated at 300 °C, 12 h, Ar- atm.

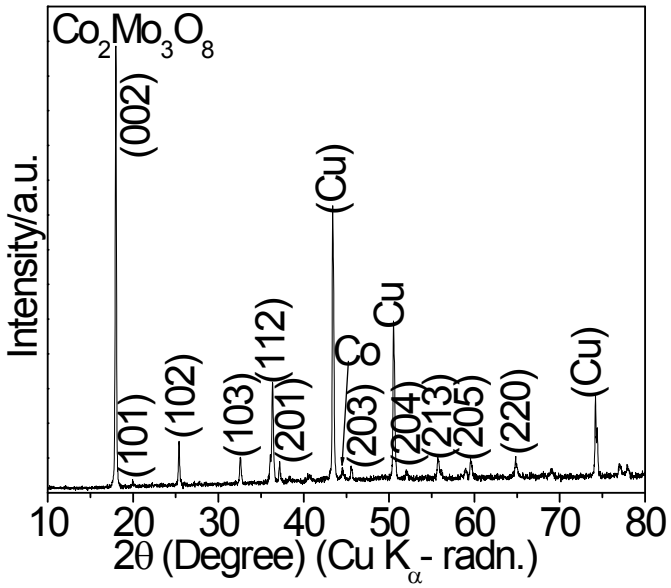

Fig. S1 X-ray diffraction patterns of $Co_2Mo_3O_8$ composite electrode heated at 300 °C, 12 h, Ar- atm. Miller indices (*h k l*) are shown. The characteristic lines due to Cu are from the current collector. Co- impurity is from the material. The y- axis values are normalized for better comparison at various voltages.

Ex-situ XRD of $Co_2Mo_3O_8$ composite electrode during 1st cycle.

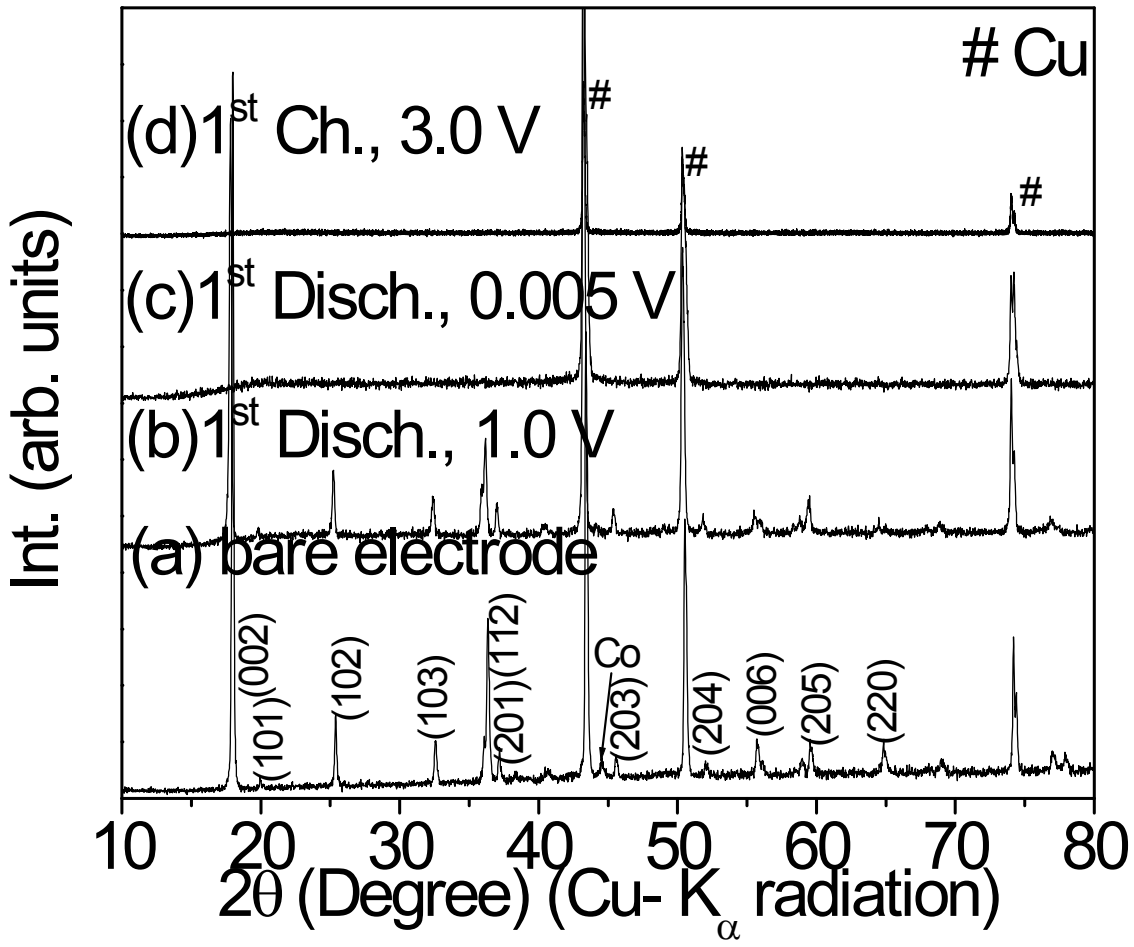

Fig. S2 X-ray diffraction patterns of $Co_2Mo_3O_8$ composite electrode. (a) Bare electrode. (b) 1st discharge; 1.0 V. (c) 1st discharge; 0.005 V. (d) 1st charge; 3.0 V. The characteristic lines due to Cu are from the current collector. Co- impurity is from the material. The y- axis values are normalized for better comparison at various voltages.

Ex-situ TEM of $Co_2Mo_3O_8$ composite electrode at 1st discharge to 0.005 V.

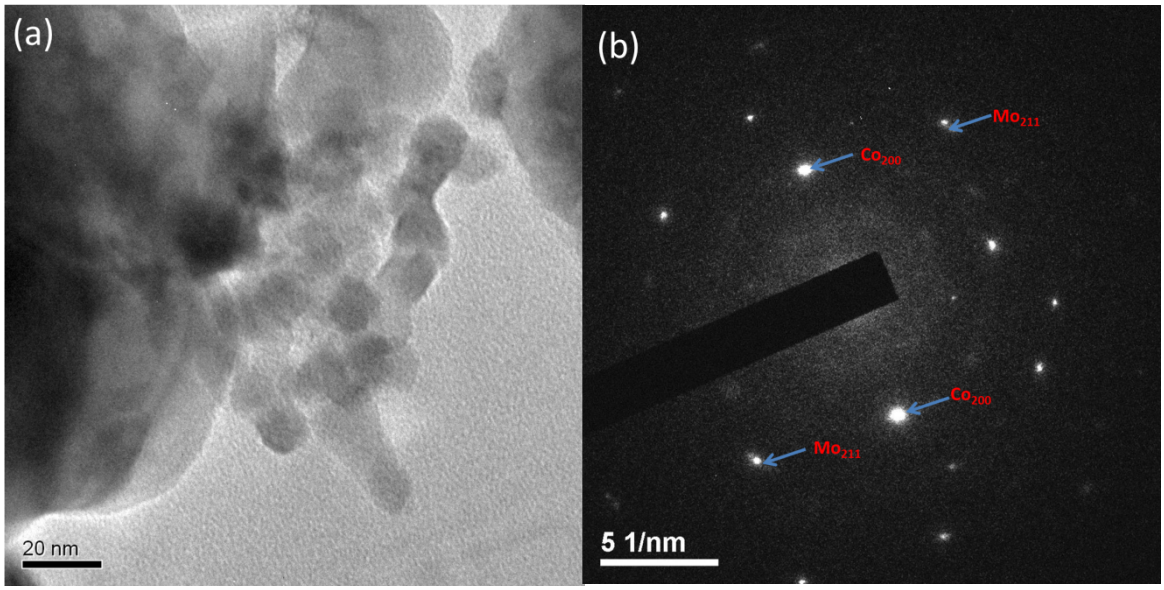

Fig. S3 Ex situ TEM for the cycled electrode (at 60 mA g^{-1}) of $Co_2Mo_3O_8$ during 1st discharge to 0.005 V. (a) TEM image and (b) SAED pattern. Scale bars are shown.

Sample preparation:

Ex-situ XRD: The composite electrode was discharged and charged during 1st 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_α 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.