

Supporting information for

Investigation on reversible metal ion (Li^+ , Na^+ , Mg^{2+} , Al^{3+}) insertion in MoTe_2 for aqueous battery

Sunny Nandi^{a,c}, Yichen Yan^b, Xintong Yuan^c, Chongzhen Wang^c, Ximin He^b, Yuzhang Li^{*c}, Shyamal

K. Das^{*a}

^aDepartment of Physics, Tezpur University, Assam 784028, India

^bDepartment of Materials Science and Engineering, University of California, Los Angeles 90095, United States

^cDepartment of Chemical and Biomolecular Engineering, University of California, Los Angeles 90095, United States

Experimental details:

MoTe_2 powder was prepared via a facile one-pot hydrothermal process adapted from a previous report [ref. S1]. In brief, 766 mg of tellurium metal (Te) powder and 700 mg of sodium borohydride (NaBH_4) were added to 5 m of DI water in an ice bath. After 30 min, a clear Te precursor was obtained. Then, 726 mg of sodium molybdate dihydrate ($\text{Na}_2\text{MoO}_4 \cdot 2\text{H}_2\text{O}$) was added to 30 ml of DI water and stir for 10 min. Then, the as-formed mixture was added to the Te precursor and stirred for another 30 min, followed by transfer of the mixture to a Teflon-lined stainless autoclave (50 ml) and heated at 200 °C for 48 hr. After cooling down to room temperature, the precipitates were collected, washed with deionized water and ethanol for three times and dried at 60 °C for 12 hr.

The crystal structure and morphology were characterized by X-ray diffraction (XRD, Rigaku Miniflex II diffractometer with $\text{Cu K}\alpha$ radiation operated at 30 kV and 15 mA), field emission electron microscopy (FESEM, ZEISS Supra 40V), and transmission electron microscopy (TEM, JEOL-2010 F). The surface chemical compositions of the samples were analyzed by X-ray photoelectron spectroscopy (XPS, AXIS Ultra DLD system). Raman spectra are recorded on a RENISHAW BASIS SERIES having 514 laser excitation. Ex-situ UV-visible spectra were recorded from Shimadzu UV-Vis

spectrophotometer for pristine MoTe₂, MoTe₂ after 1st/10th/50th discharge states in 1 M AlCl₃ aqueous electrolyte. Electrode slurry was prepared by mixing the active material (MoTe₂), carbon black and PVDF in a weight ratio of 80:10:10 using N-methyl-2-pyrrolidone solvent. The slurry was drop cast on a carbon cloth (14mm in diameter, Fuel cell store, USA, ELAT hydrophilic, Product code: 1591002) and dried at 60 °C for 12 hr.

Cyclic voltammetry (CV) and galvanostatic discharge/charge experiments were conducted in a conventional three-electrode electrochemical glass cell where a Pt electrode and Ag/AgCl electrode were used as the counter and reference electrodes, respectively. The discharge/charge and CV experiments were performed in a voltage range of -0.7 to 0.8 V (vs. Ag/AgCl). Electrochemical impedance spectra (EIS) were recorded in frequency range of 1 mHz-200 kHz at 10 mV signal amplitude. All the electrochemical tests were performed at room temperature (25 °C)

Reference:

S1: L. Ding, J. Wei, Y. Qiu, Y. Wang, Z. Wen, J. Qian, N. Hao, C. Ding, Y. Li and K. Wang, *Chem. Eng. Journal*, 2021, **407**, 127213.

Supplementary figures

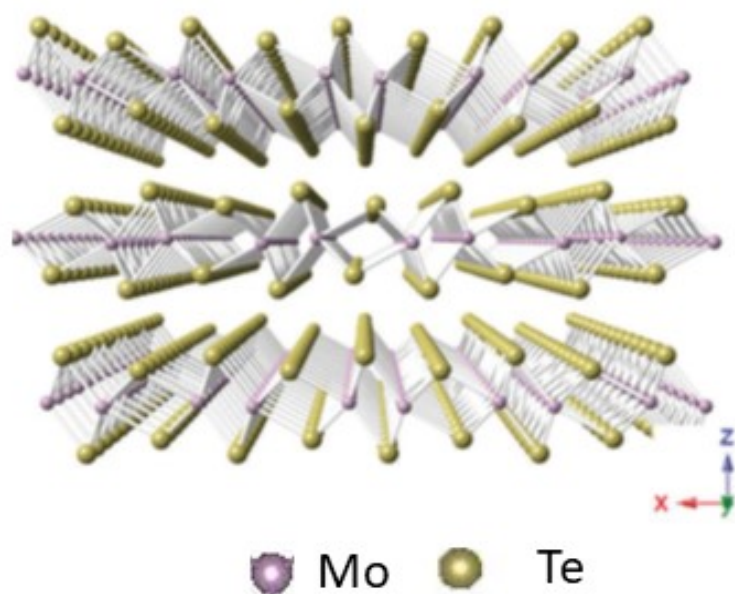


Figure S1: Crystal structure of MoTe₂. Reproduced with permission from ref [7b], copyright 2018

Wiley Journal.

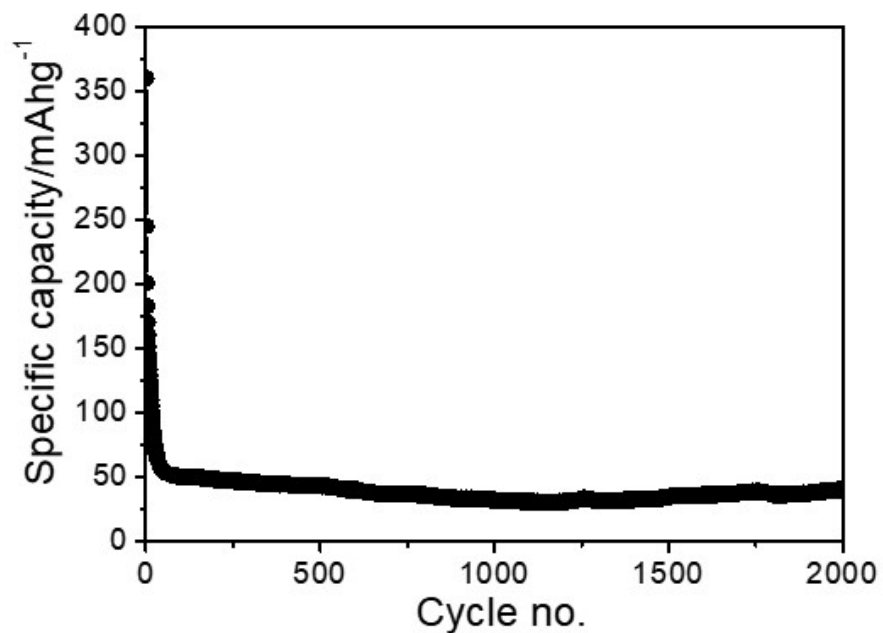


Figure S2: Variation of discharge capacities with cycle in 1 M AlCl_3 aqueous electrolyte at a current density of 5 Ag^{-1} .

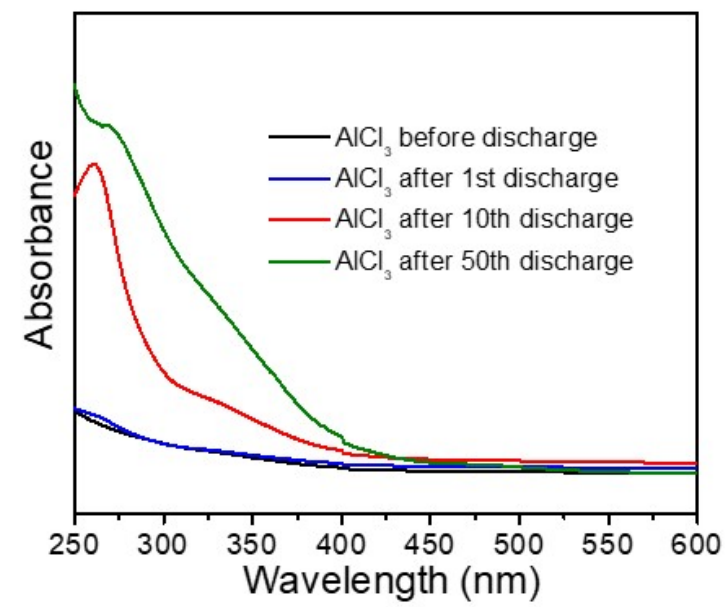


Figure S3: UV-visible spectrum of the aqueous electrolyte before and after 1st, 10th and 50th discharge cycles.

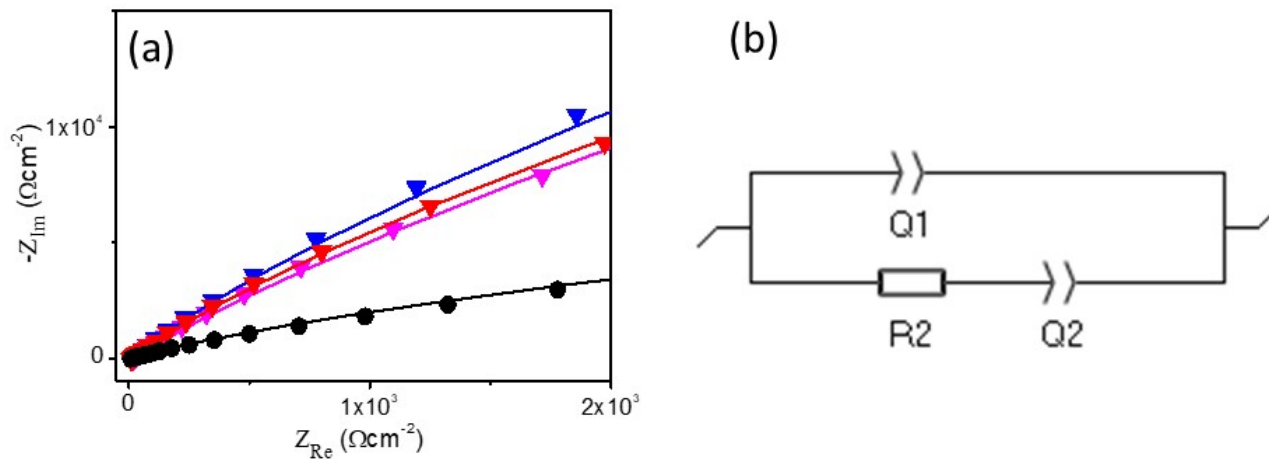


Figure S4: (a) Enlarged region of the EIS fitted data as shown in Figure 3f. (b) Circuit diagram of the equivalent circuit used to fit the experimental data. Here $R2$ corresponds to the charge transfer resistance.

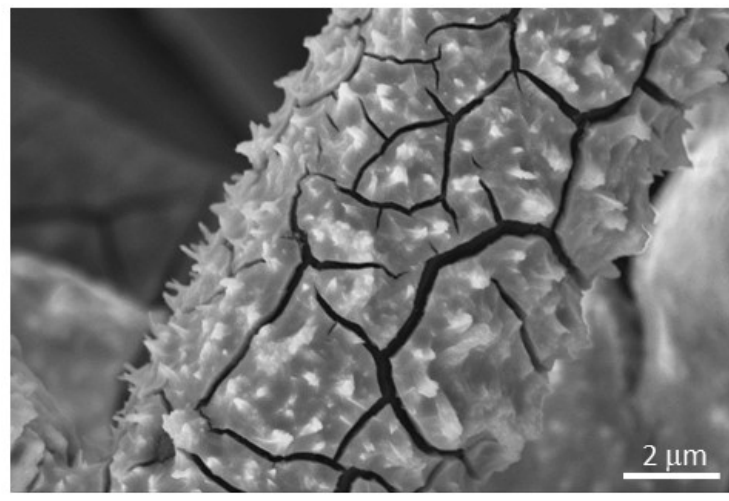


Figure S5: ex-situ FESEM image of MoTe₂ after the 1st charge state.

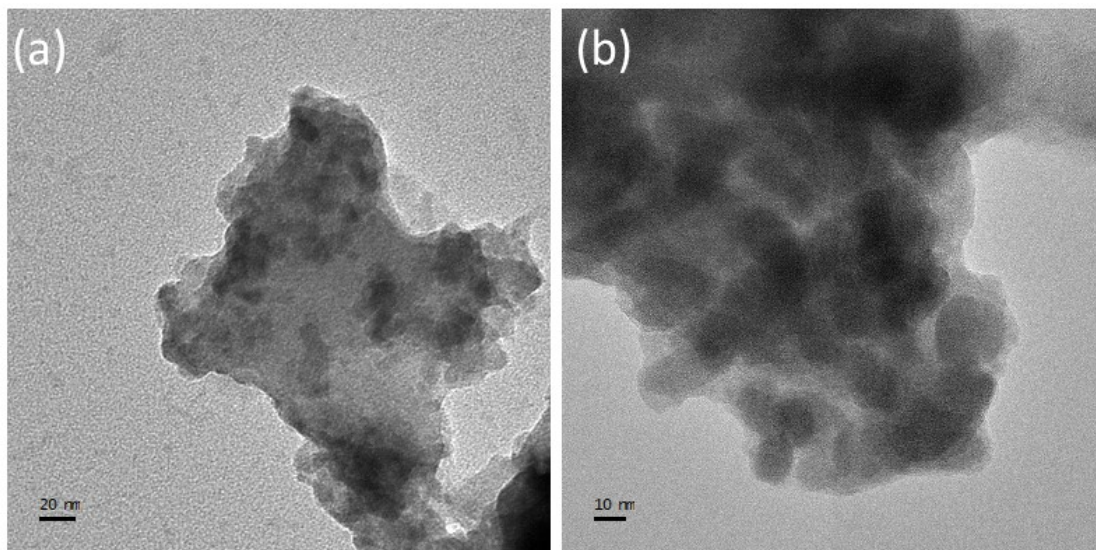


Figure S6: ex-situ TEM images of MoTe₂ after the 1st discharge state.

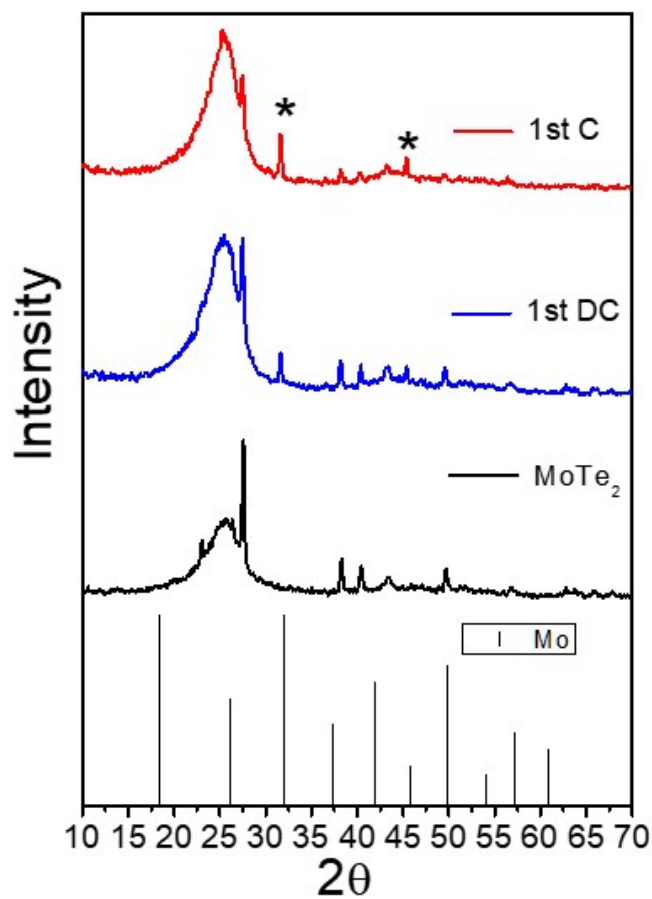


Figure S7: ex-situ XRD patterns of MoTe₂ before and after 1st discharge/ 1st charge state in 1 M NaCl aqueous electrolyte. * marked peaks refer to Mo.

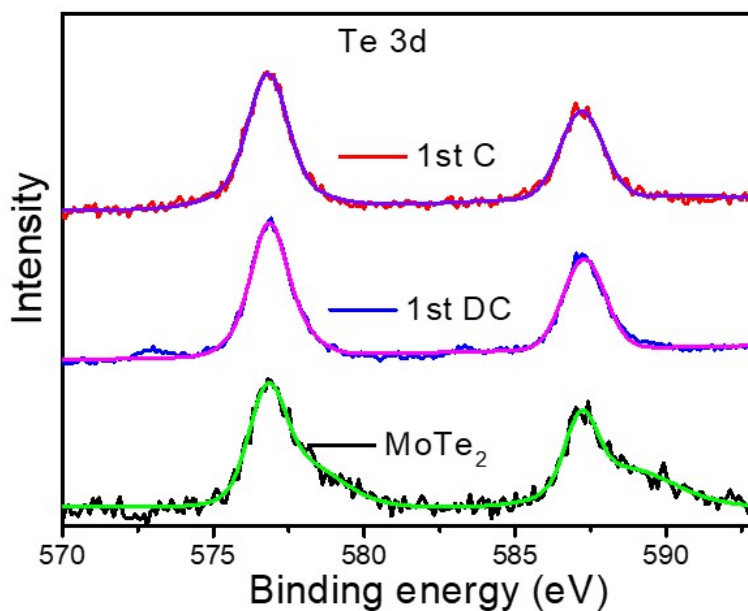


Figure S8: ex-situ XPS spectra of Te 3d before and after 1st discharge/ 1st charge state respectively.

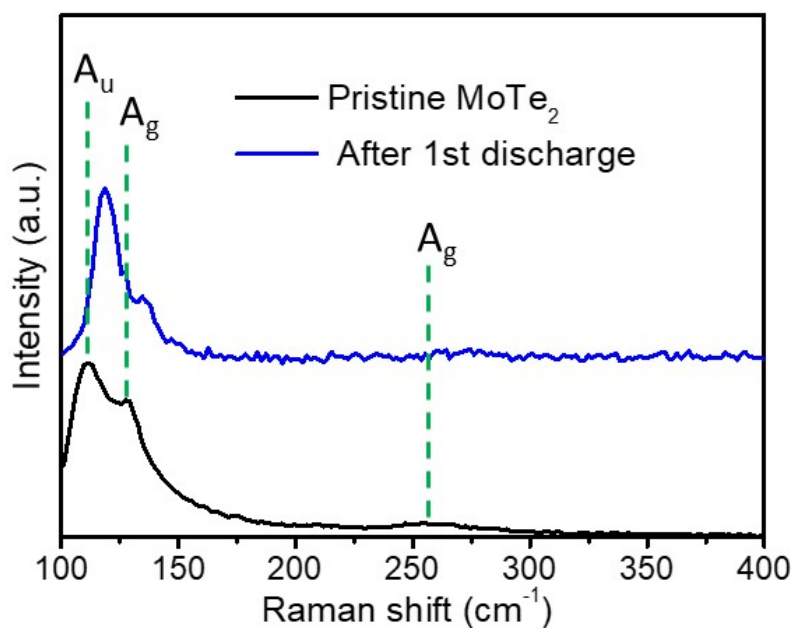


Figure S9: ex-situ Raman spectra of MoTe₂ before and after 1st discharge in 1 M AlCl₃ aqueous electrolyte. The dotted lines represent the characteristic peaks of MoTe₂.

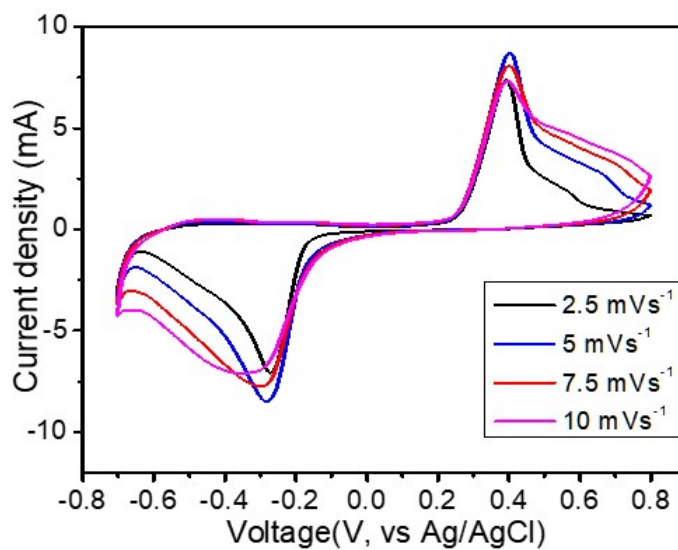


Figure S10: CV curves of MoTe₂ at different scan rates in 1 M AlCl₃ aqueous electrolyte.

Table S1: Charge transfer resistance values obtained from fitting the data shown in figure S4

Sl no.	Electrolytes	Charge transfer resistance (R ₂) (ohm cm ⁻²)
1.	1 M AlCl ₃	8.79
2.	1 M MgCl ₂	9.29
3.	1 M NaCl	12.9
4.	1 M LiCl	17.9