

Supplementary Material

Correlation of crystal structure and ion storage behavior of MoO₃ electrode materials for aluminum-ion energy storage studied with in-situ X-ray spectroscopies

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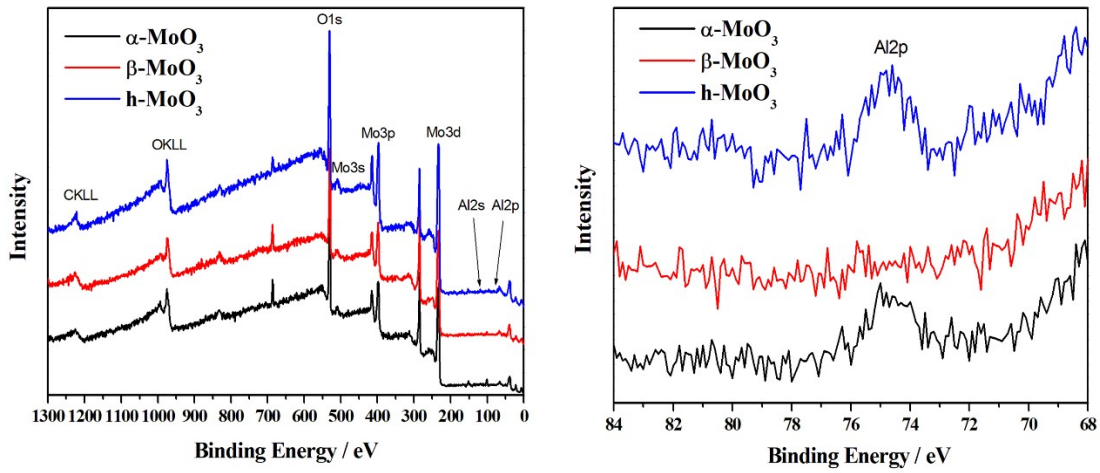


Figure S1. The XPS spectra of the MoO₃ materials with various crystal phases after insertion of Al³⁺ ion.

Table S1. As-characterized composition of the MoO₃ electrodes with various crystal phases after insertion of Al³⁺ ion deduced by XPS measurements.

Sample	Al atomic content %	Mo atomic content %	O atomic content %
α -MoO ₃	1.33	19.07	79.59
β -MoO ₃	0.14	21.92	77.94
h -MoO ₃	0.98	20.99	78.09

The Electrochemical impedance spectroscopy (EIS) measurements of the various MoO₃ electrode materials are shown in Figure S2. The EIS measurements were recorded in a frequency range of 10⁵ to 0.1 Hz at an open circuit potential. In the high-frequency region of Nyquist plots, the intersection with real axis and the diameter of semicircle represent the resistance of electrochemical system (R_s) and charge transfer resistance (R_{ct}), respectively. There clearly show smaller R_{ct} for the α -MoO₃ and h -MoO₃ electrode materials, whereas the β -MoO₃ electrode material has the largest R_{ct} . This result indicates that the charge-transfer at the interface for the α -MoO₃ and h -MoO₃ electrode materials is relatively easier than that for β -MoO₃. Furthermore, the slope of straight line in the low-frequency region is defined as the diffusion resistance. The slope trend (α -MoO₃ > h -MoO₃ and β -MoO₃) indicates that the diffusion resistance of α -MoO₃ is lower than that of h -MoO₃ and β -MoO₃, whereas the diffusion resistances of both h -MoO₃ and β -MoO₃ electrode materials show no significant difference.

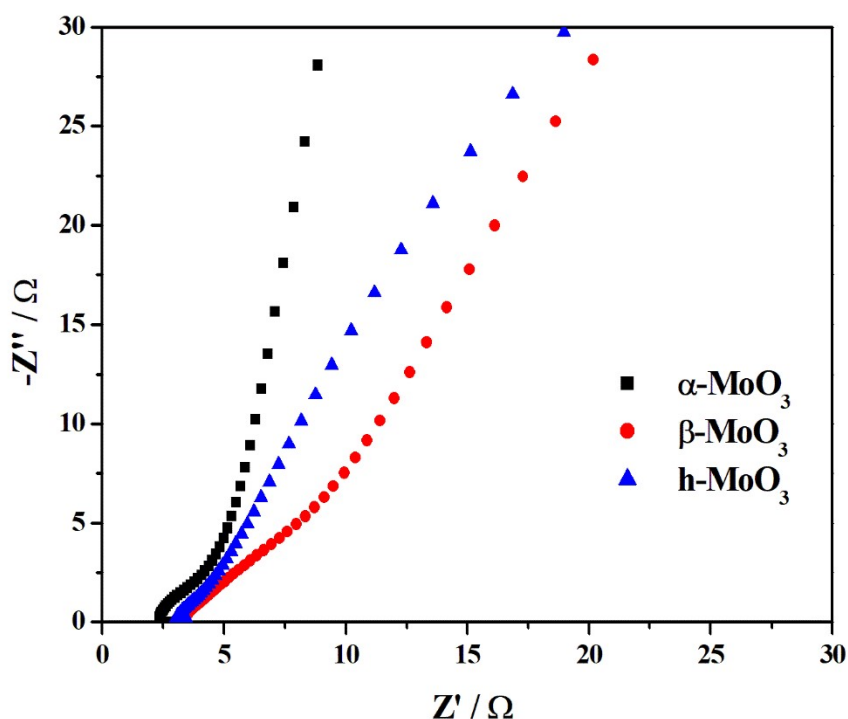


Figure S2. The EIS curves of various MoO₃ electrode materials.

The rate performance of the various MoO_3 electrode materials is characterized under current density from 1 A g^{-1} to 5 A g^{-1} with potential range from -0.7 V to 0.6 V . It is observed that the charge and discharge gravimetric capacities are decreased with increasing current density, which is attributed to the polarization phenomenon of the MoO_3 electrode materials.

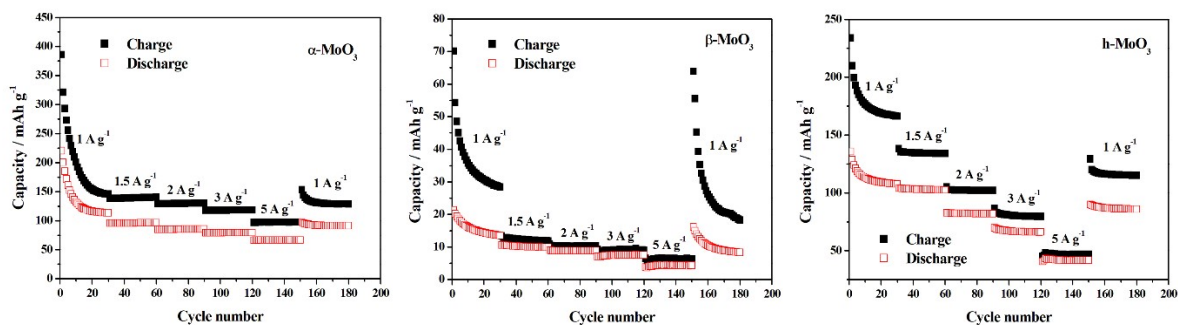


Figure S3. Rate performance and variation of charge/discharge capacities of the various MoO_3 electrode materials.

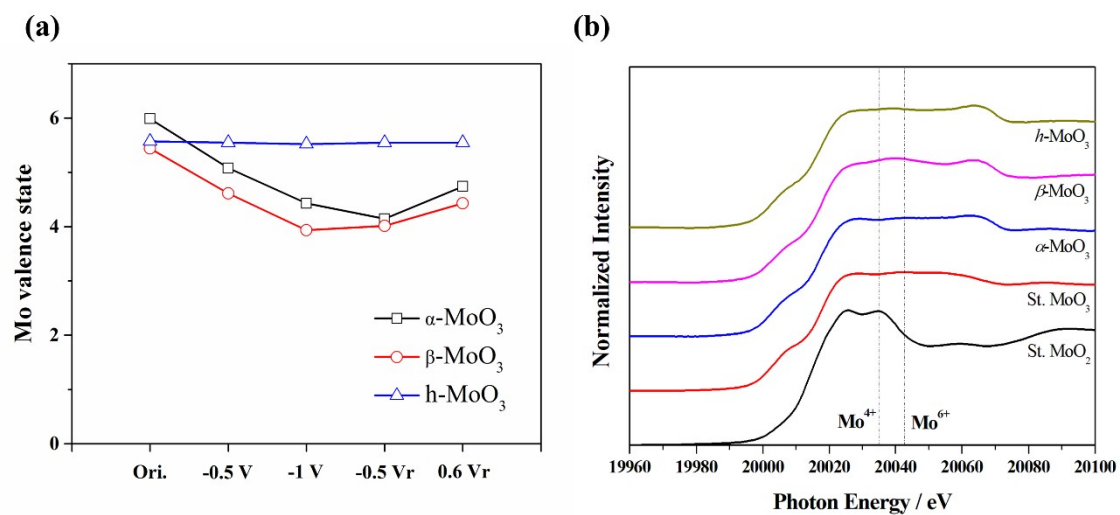


Figure S4. (a) The average valence state of Mo in the various MoO₃ electrode materials under insertion/extraction of Al³⁺ ion, and (b) the Mo K-edge XANES spectra of the various MoO₃ electrode materials together with the reference samples.

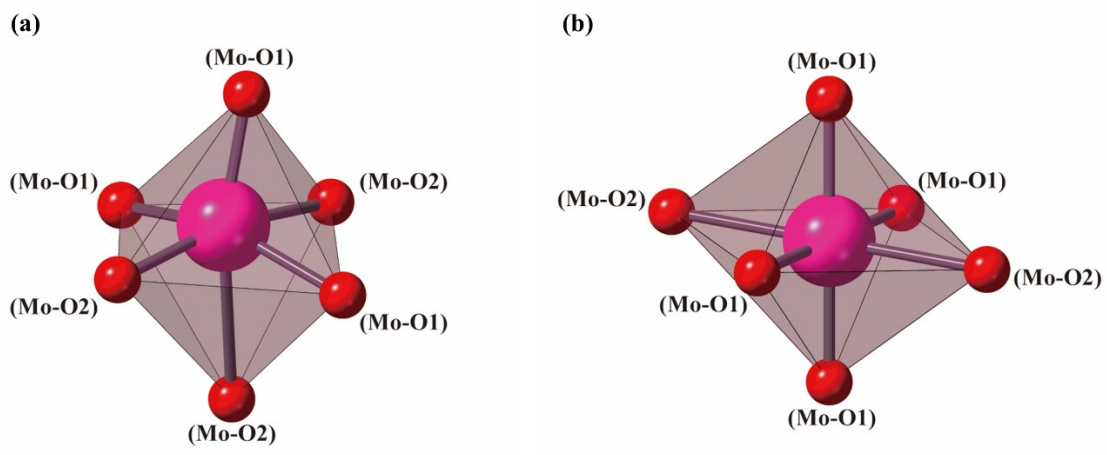


Figure S5. The MoO_6 octahedral structure in the (a) $\alpha\text{-MoO}_3$, and (b) $\beta\text{-MoO}_3$ materials.