Nanoscale

Supporting Information

Direct Conversion of Multilayer Molybdenum Trioxide to Nanorods as Multifunctional Electrodes in Lithium-Ion Batteries

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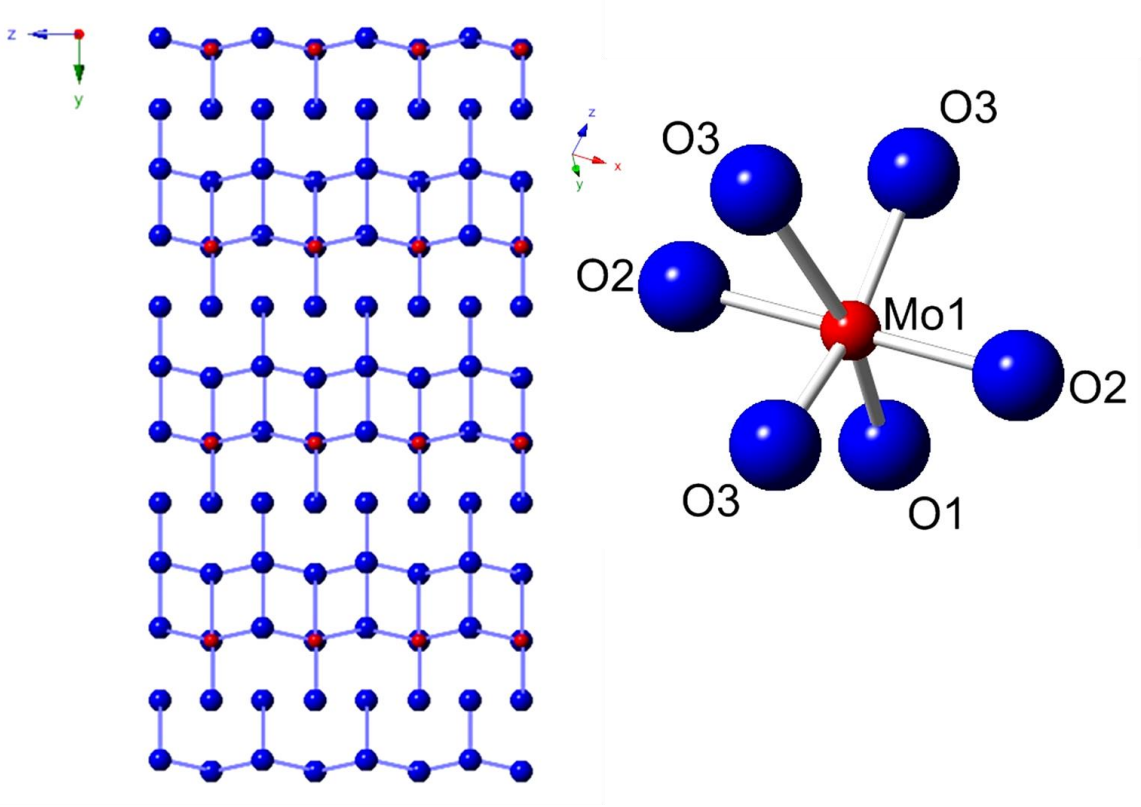


Figure S1. Crystal structure model of MoO_3: The (100) section of the crystal structure model of MoO_3 and MoO_6 supercell; blue and red balls represent O and Mo atoms, respectively. The structure of MoO_3 is anisotropic; it can be considered as a layered structure parallel to (010). Each layer comprises two sublayers, each of which is formed by corner-shared octahedra along [001] and [100]; the two sublayers stack together by sharing the edges of the octahedra along [001]. Here, the calculated lattice parameters *a*, *b*, and *c* are 3.92, 13.94, and 3.66 Å, consistent with the standard data recorded in CPDS #35-0609.

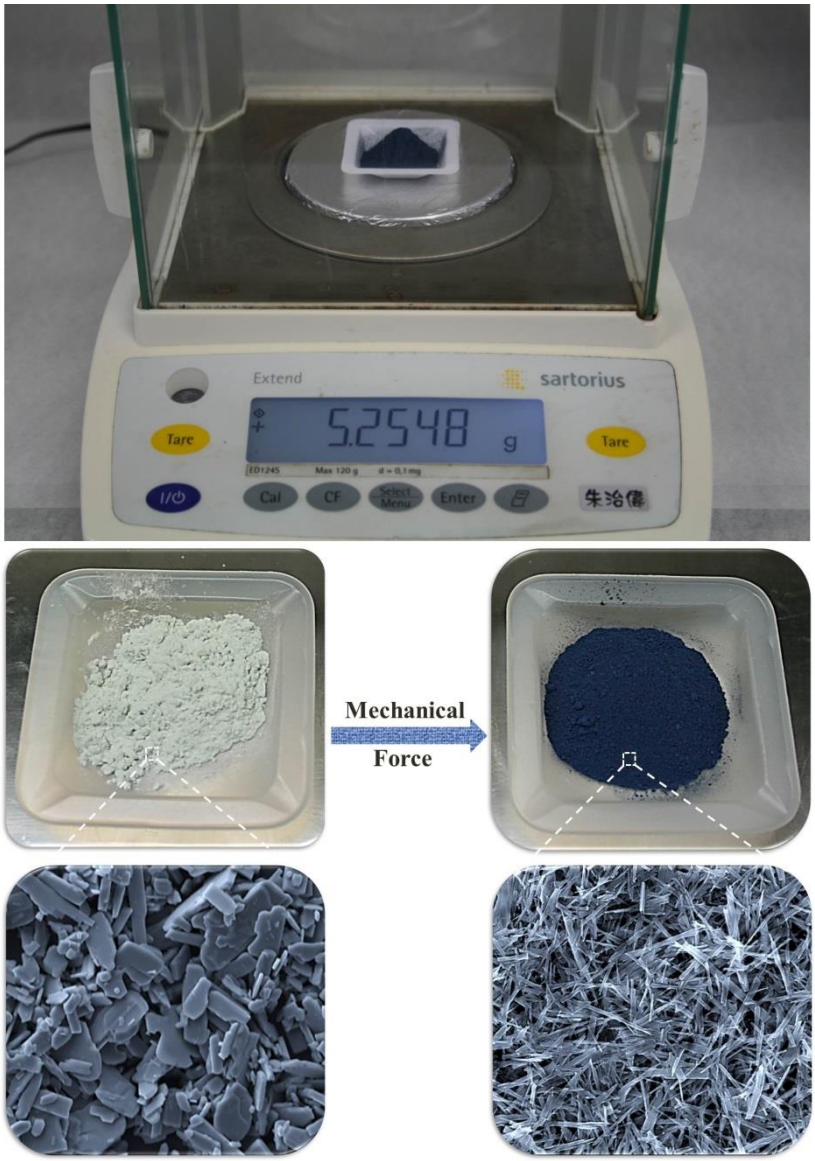


Figure S2. High yield of MoO_3 nanorods: Photograph of a powder of MoO_3 nanorods produced in a large quantity (ca. 5.25 g). This method can be scaled-up readily to produce large quantities (grams) of dispersions or powders. This powder sample was prepared at an initial concentration of 5 wt% and a grinding time 90 min. This method has the advantage of allowing large amounts (ca. 2 g) of product to be prepared in a single batch. The beneath images are the bulk and nanorods powders with their crosspondance SEM images.

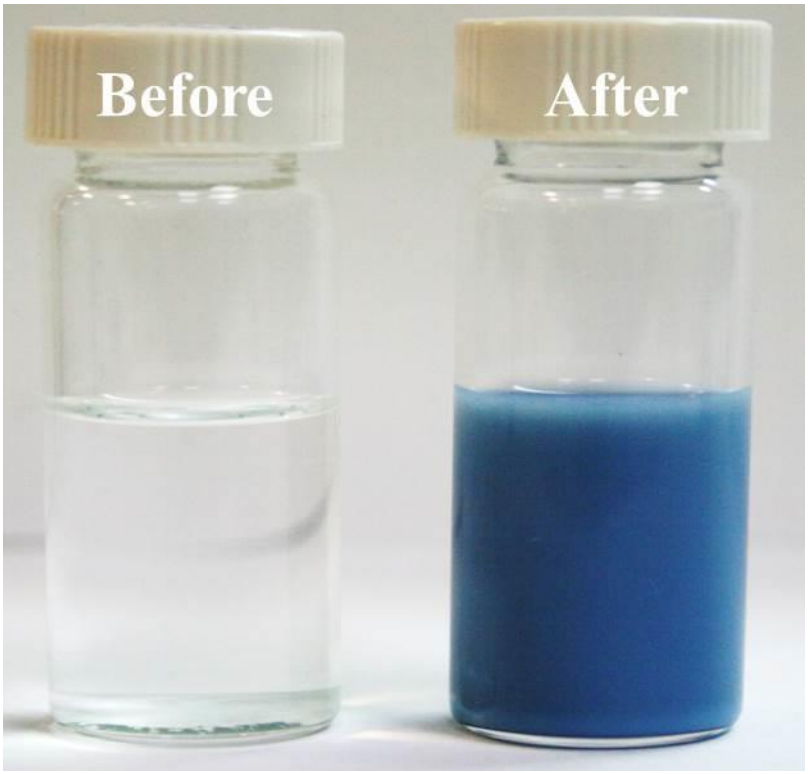


Figure S3. Sedimentation test: MoO_3 dispersions (2.5 mL) before and after grinding for 90 min in IPA (initial concentration: 5 wt %). Sedimentation tests were performed by storing dispersions (prepared before and after grinding) in IPA for more than three months. The material prepared without grinding precipitated completely (bottom of the vial on the left-hand side) after several minutes, but the dispersion of MoO_3 nanorods was highly stable without any precipitation. Thus, the grinding process increased the compatibility of the nanomaterials with the solvent, increased the repulsive forces among the nanorods, and prevented the materials from undergoing serious aggregation.

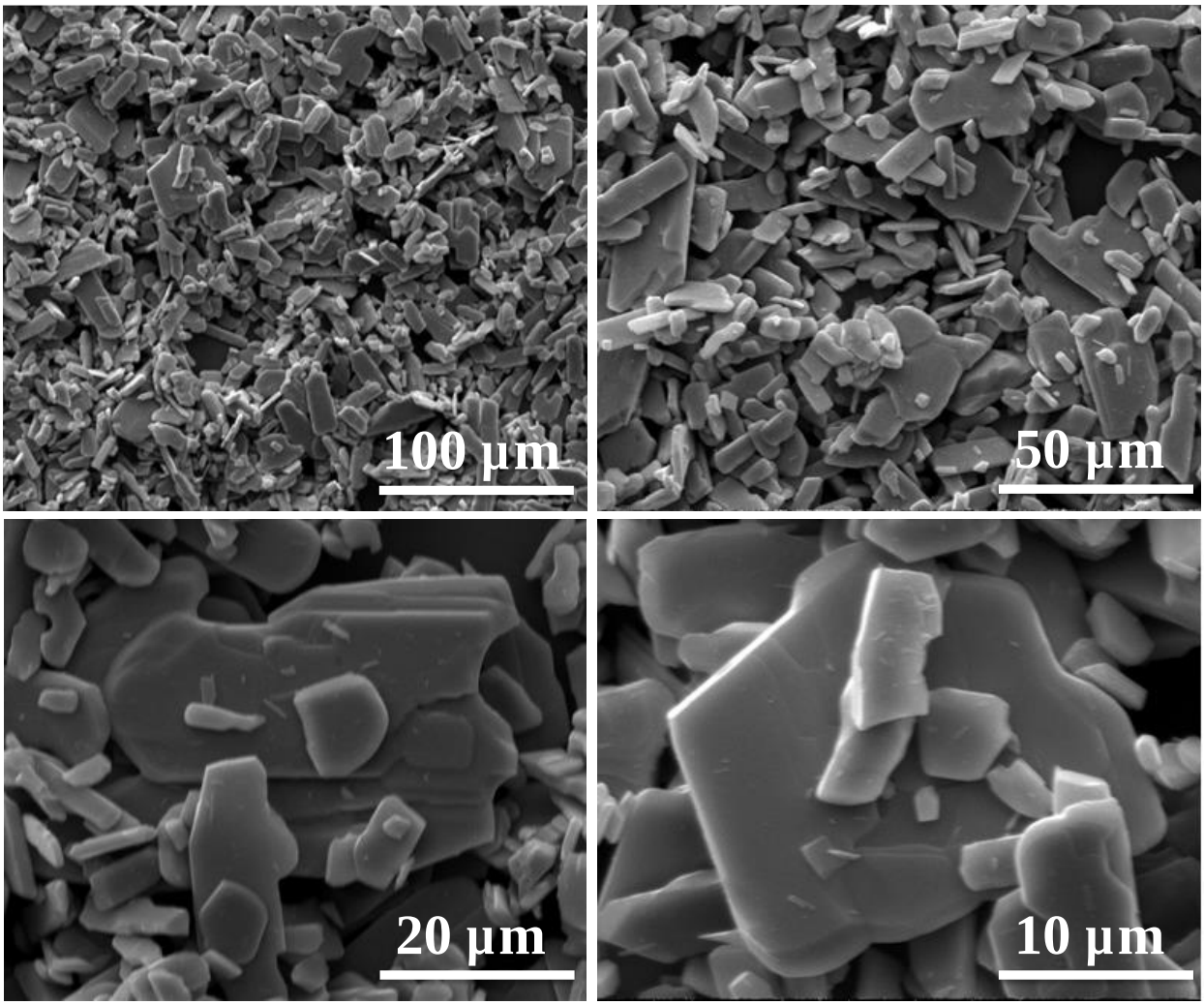


Figure S4. Morphology of pristine MoO_3 materials: SEM images of 3D pristine network MoO_3 materials at various scale ranges. The materials feature a highly arranged layer-by-layer structure, with single sheets having large lateral dimensions (>10 µm) and thicknesses of greater than 2 µm.

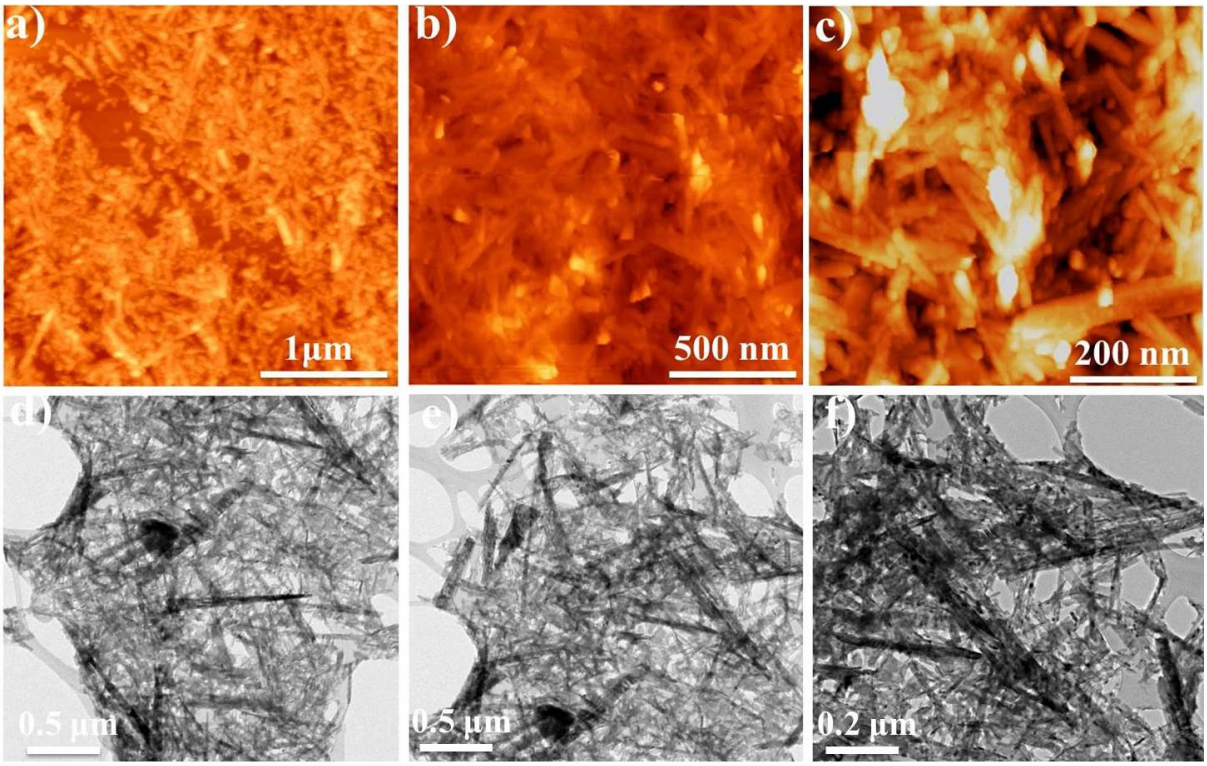


Figure S5. Morphology of the resultant MoO_3 nanorods: (a–c) AFM height images and (d–f) TEM images, displayed at various scales, of a sample ground for 90 min.

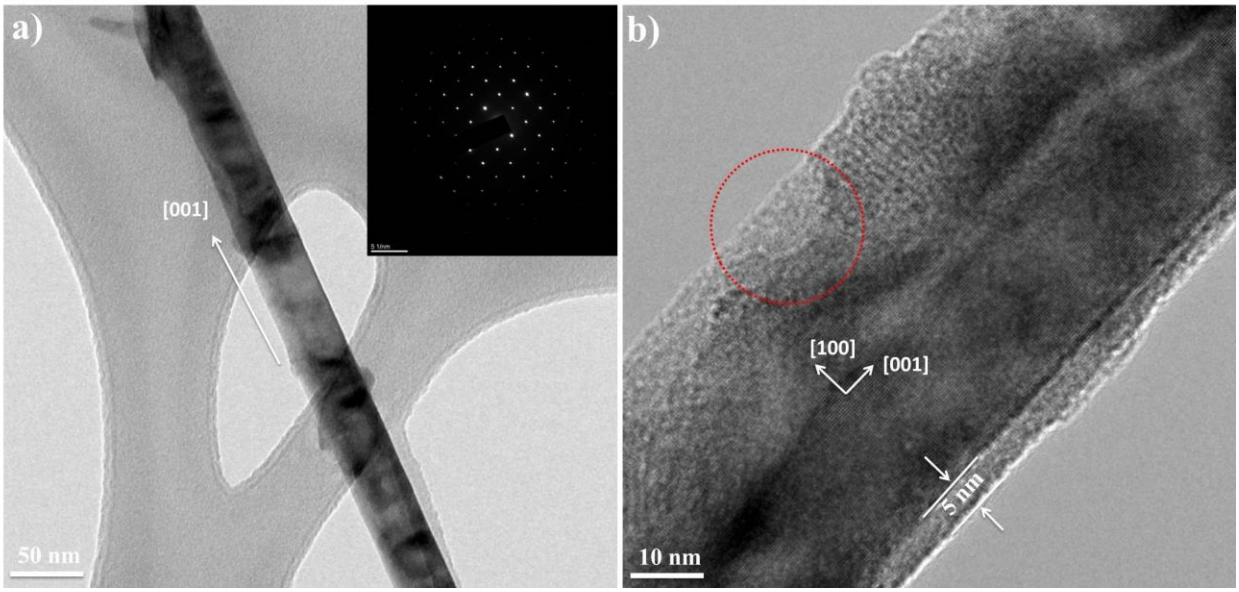


Figure S6. TEM analysis of a MoO_3 nanorod: (a) TEM image of a typical nanorod (inset: corresponding SAED pattern) and (b) HRTEM image of a flattened area of the sample in (a). The direction of fracturing is displayed by the arrow in (a); the step-like edge of the nanorod is displayed by the red circle in (b).

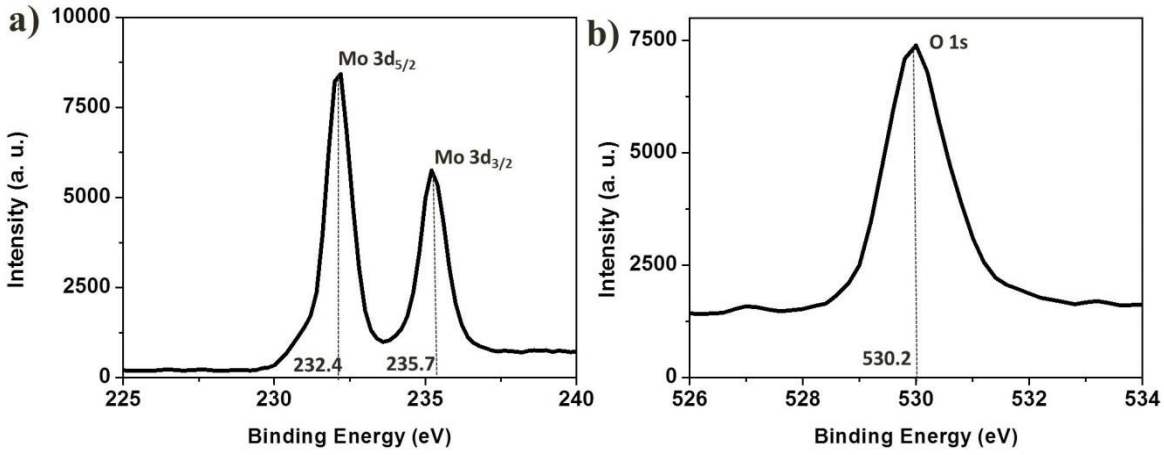
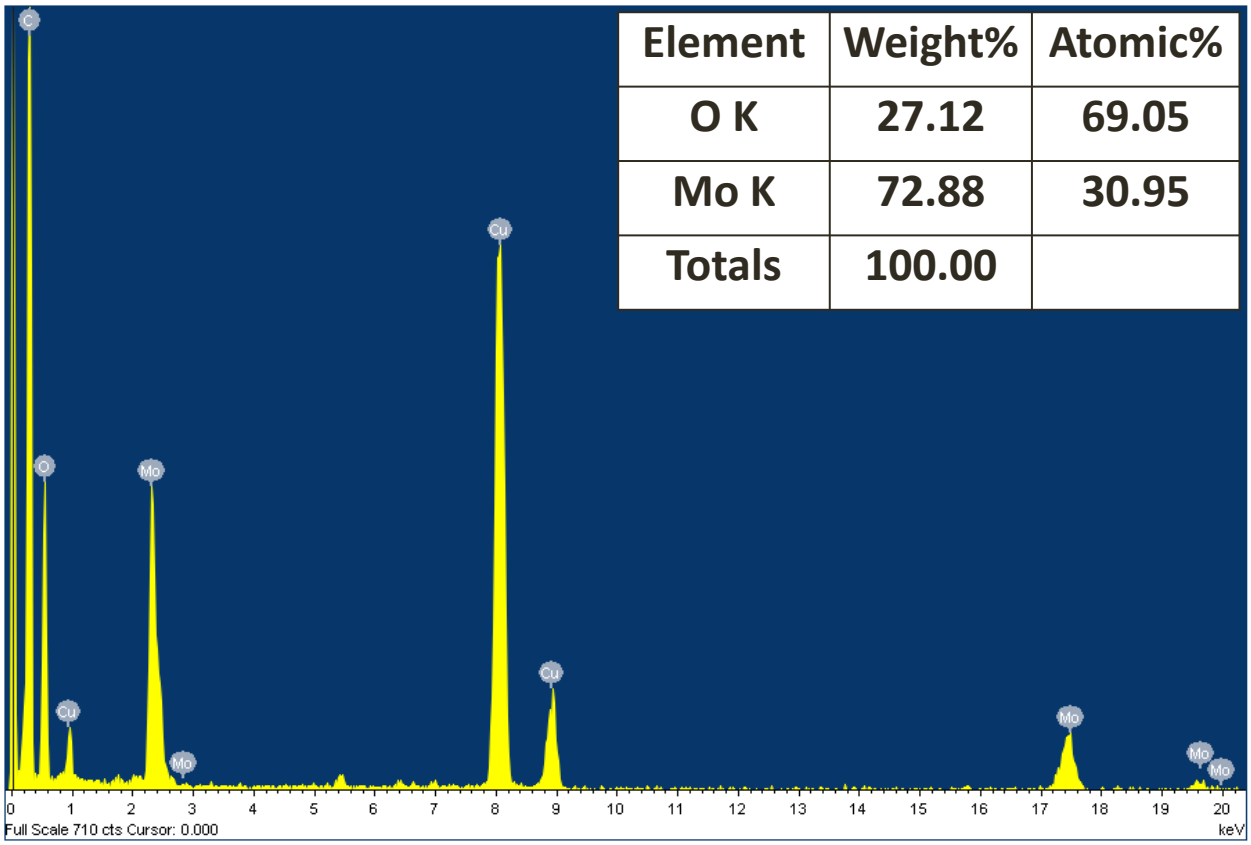


Figure S7. XPS spectra of MoO_3 nanorods: XPS data of the binding energies (BEs) of (a) Mo 3d and (b) O 1s atoms in MoO_3 nanorods. The peaks at 242.4 ± 0.1 and 235.7 ± 0.1 eV can be assigned to the Mo $3d_{5/2}$ and Mo $3d_{3/2}$ orbitals, respectively; that at a BE of 530.2 ± 0.1 eV represents the O 1s orbital of MoO_3. The stoichiometry of MoO_3 was confirmed from the Mo:O atomic ratio of 1:3.



Element	Weight%	Atomic%
O K	27.12	69.05
Mo K	72.88	30.95
Totals	100.00	

Figure S8. Compositional analysis of MoO_3 nanorods: Energy-dispersive X-ray analysis (EDS) of MoO_3 nanorods; inset: Table revealing the Mo:O atomic ratio to be 1:3, in agreement with the stoichiometric ratio of MoO_3. Signals for Cu atoms arose from the holey carbon-coated copper grid.

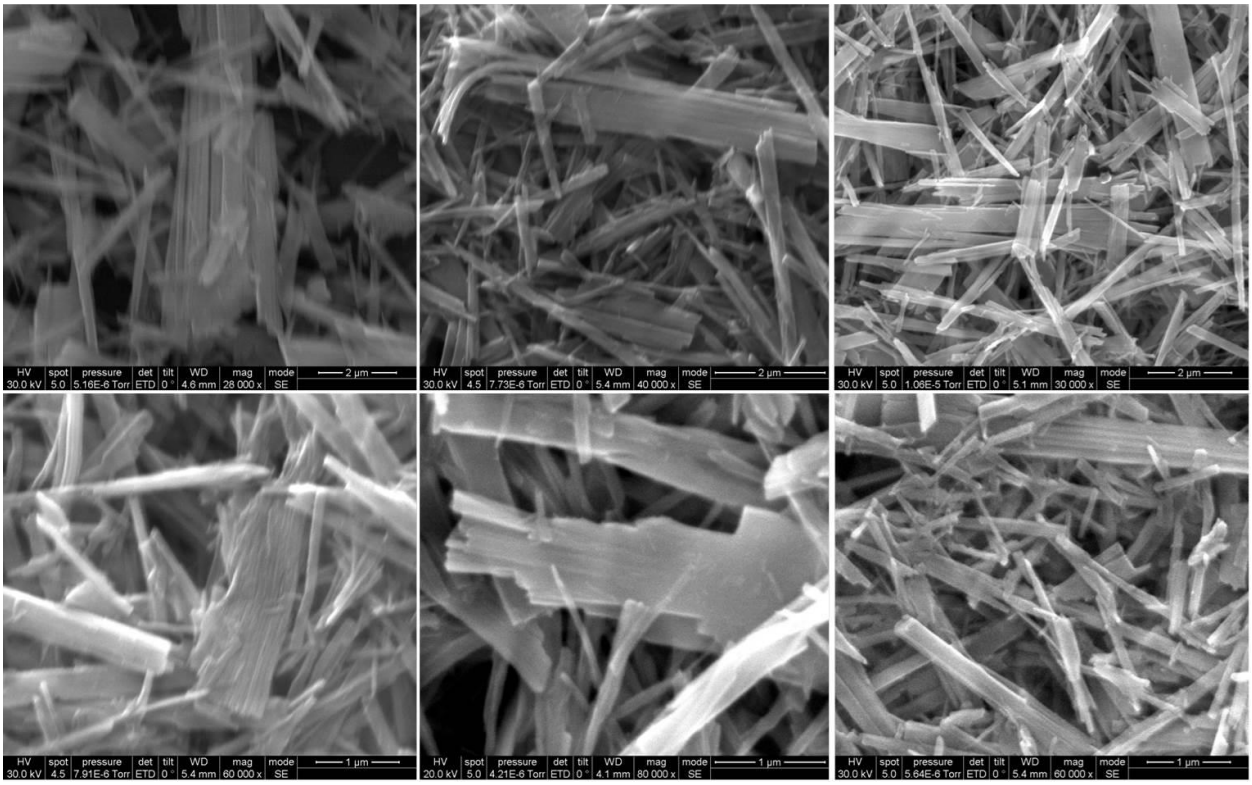


Figure S9. Library of 2D fractured MoO_3 samples at various scales: SEM images of the fractured MoO_3 sample obtained during the intermediate stages of the conversion process.

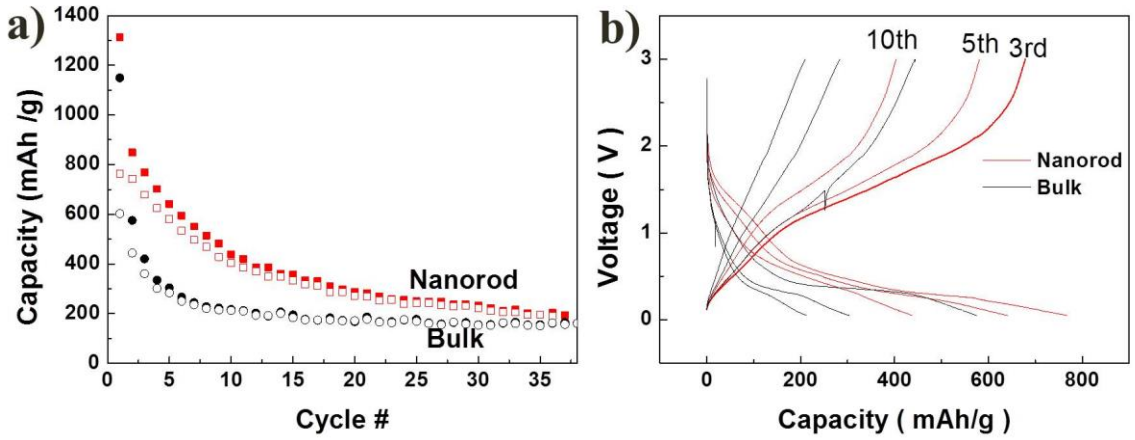


Figure S10. MoO_3 anode electrodes in lithium-ion battery: (a) Cycling performance at a constant current rate 50 mA g^{-1} for nanorods and bulk MoO_3 samples. (b) Charge/discharge voltage profiles at 50 mA g^{-1}; rate behavior at various current rates.