Supplementary Material (ESI) for Chemical Communications

Electronic Supplementary Information for:

Superior stability and high capacity of restacked molybdenum disulfide as anode material for lithium ion batteries

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Characterization details

The samples were characterized by transmission electron microscopy (TEM, JEOL 2011, 200 keV), X-ray diffraction (XRD, Philips PW1730 diffractometer with Cu Kα radiation, λ = 1.54056 Å), and Raman spectroscopy (Jobin Yvon HR800). The XRD profiles were refined by the program Fullprof. Specific surface area was determined by gas adsorption on NOVA 1000 (Quantachrome). Magnetic measurements were performed using a conventional physical properties measurement system (PPMS). Magnetic hysteresis loops were performed at room temperature with fields up to 1T. Electrochemical measurements were carried out using a 2032-type coin cell fabricated in an Ar-filled glove box (Mbraun, Germany). The working electrode was 70:20:10 (w/w) active material/carbon black/polyvinylidene difluoride, and lithium foil served as counter and reference electrode. The electrolyte was 1 M $LiPF_6$ dissolved in 1:2 ethylene carbonate (EC) and diethyl carbonate (DEC). The constant current charge/discharge cycling was conducted on a LAND battery tester (CT2001A) in the voltage range between 3.0 and 0.01 V. The cyclic voltammetry (CV) was performed on a CHI660C electrochemical workstation at a scan rate of 0.2 mV s^{-1}. The electrochemical impedance spectroscopy (EIS) was conducted on a Parstat 2273 potentiostat/galvanostat analyzer (Princeton Applied Research & AMTECH Company) with an amplitude of 5 mV in the frequency range from 10 mHz to 100 kHz. Prior to the EIS measurements, the cells were run for 5 cycles and then discharged to 1.6 or 0.9 V vs. Li^+/Li and held for 2 h at 25, 35, 45, or 55 ^oC.

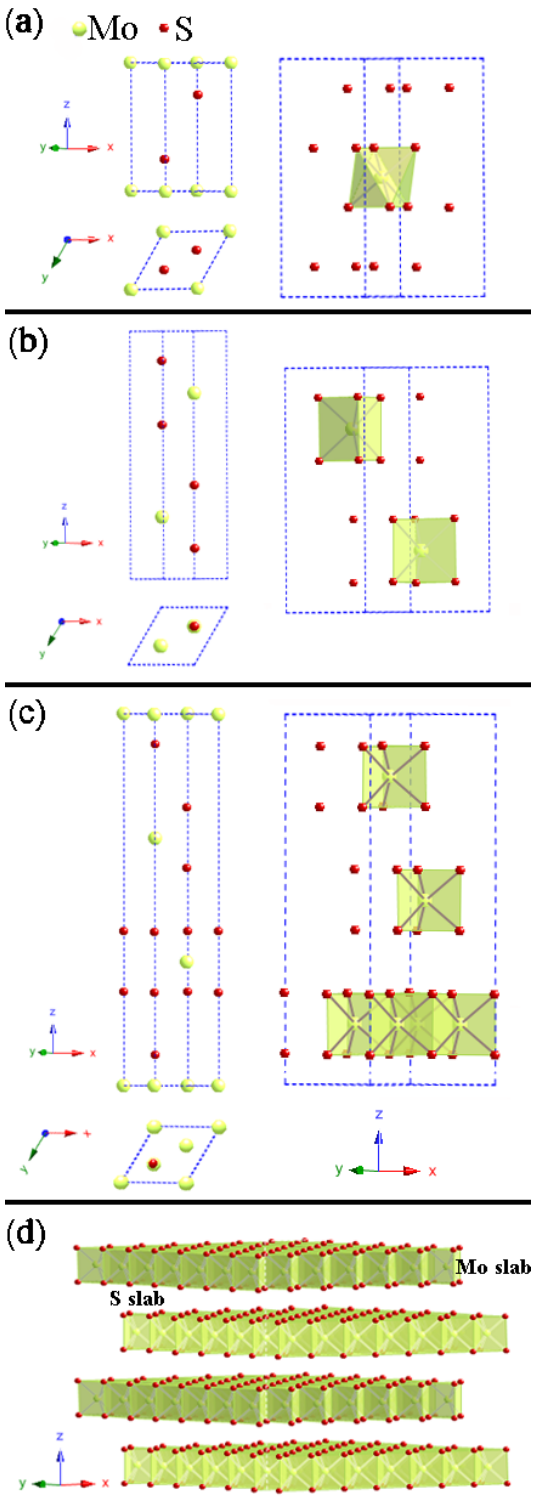

Fig. S1 Crystal structures of MoS_2 polytypes: (a) 1T, (b) 2H, (c) 3R (left: unit cell; right: $2a \times 2a$ polyhedral supercell); (d) the 2H polytype consists of Mo and S layers.

1T-MoS_2 has octahedral coordination of the molybdenum center with one Mo atom per unit cell; 2H-MoS_2 has trigonal prismatic coordination and two S-Mo-S units per unit cell; and 3R-MoS_2 also has trigonal prismatic coordination around the molybdenum atom with three S-Mo-S units per unit cell. Both the 2H and 3R polytypes have the same lattice parameter a ($b = a$)