

Atomic Scale Recognition of Structure in the Intercalation of Sodium by Aberration-Corrected Scanning Transmission Electron Microscopy

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Nowadays, the most challenging issues concerning the rechargeable batteries (e.g. sodium-batteries, etc.) are to discover new active materials and develop new techniques to increase the energy density and cycle life of the existing materials for batteries. Therefore, we focus on several materials of sodium-batteries by using aberration-corrected scanning transmission electron microscopy (STEM).

Ti₃C₂X is a functionalized two-dimensional transition-metal carbonitride [1]. As shown in Figure 1, the STEM studies show that the functional groups (e.g., OH⁻, F⁻, O⁻) and the intercalated sodium ions prefer to stay on the top sites of the centro-Ti atoms and the C atoms of the Ti₃C₂ monolayer, respectively. On the basis of the STEM observations, the previous monolayer surface model of Ti₃C₂X is modified as shown in Figure 1.

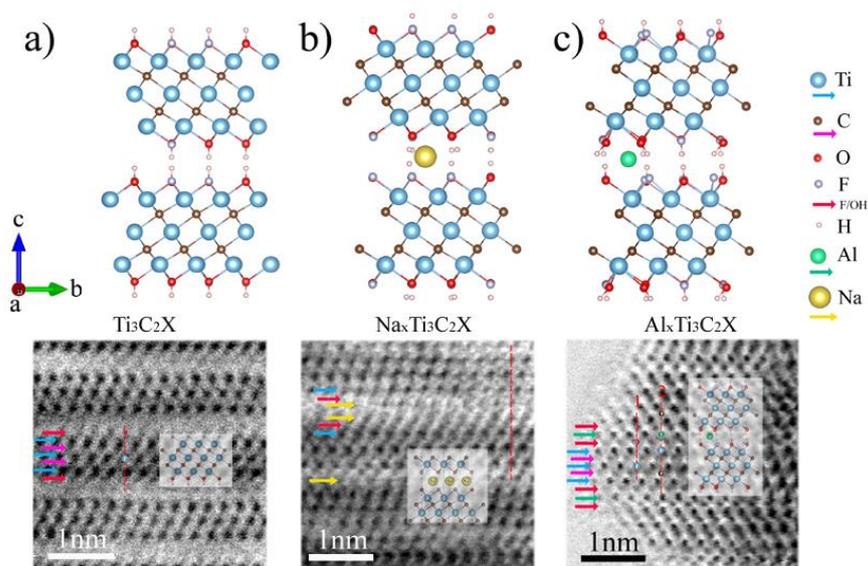


Figure 1. Optimized geometries of Ti₃C₂X (a), Na_xTi₃C₂X (b), Al_xTi₃C₂X (c) from cross-sectional view and corresponding ABF images.

The distinctive electronic and chemical properties of two-dimensional transition-metal dichalcogenide MoS₂ are closely related to the structure and intercalation chemistry [2]. Herein, the controversial phase transition from semiconductive 2H to metallic 1T phase and occupancy of the intercalated sodium upon electrochemical sodium intercalation into MoS₂ are clarified at the atomic scale in Figure 2. In addition, irreversible structural decomposition is recognized in MoS₂ depending on the content of sodium ions intercalation.

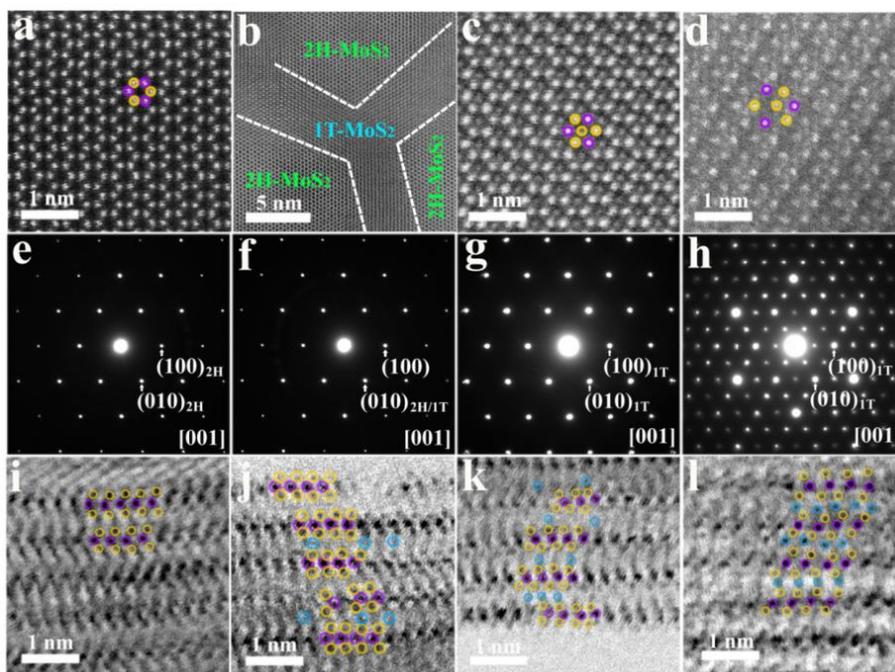


Figure 2. High-angle annular dark-field, and selected area electron diffraction images of commercial MoS₂ in Cell-60 (a and e), Cell-80 (b and f), Cell-160 (c and g), and Cell-256 (d and h) along the [001] zone axis and the annular bright field images of as-prepared nano-MoS₂ (i) with cutoff at 1.0 V (j), 0.8 V (k), and 0.2 V (l) along the [100] zone axis.

Besides, on the basis of comprehensive structural characterization, the reversibility of the conversion reaction in fully discharged MoS₂ is clarified. Either as an intermediate product or as general recharge product, NaMoS₂ is detected and recognized as a new phase in the recharged composite [3].

Reference:

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2. X. F. Wang, **X. Shen**, Z. X. Wang*, R. C. Yu*, and L. Q. Chen, Atomic-scale clarification of structural transition of MoS₂ upon sodium intercalation, ACS Nano, 2014, 8(11): 11394-11400.
3. S. Hao, **X. Shen**, M. Tian, R. C. Yu*, Z. X. Wang*, and L. Q. Chen, Reversible conversion of MoS₂ upon sodium extraction, Nano Energy, 2017, 41: 217-224.