Electronic Supplementary Material (ESI) for Nanoscale. This journal is © The Royal Society of Chemistry 2016

Electronic Supplementary Information

Conversion of 1T-MoSe₂ to 2H-MoS_{2x}Se_{2-2x} mesoporous nanospheres for superior sodium storage performance

Junjun Zhang,^{ab1} Wenpei Kang,^{bd1} Miao Jiang,^a Yu You,^a Yulin Cao,^e Tsz-Wai Ng,^b Denis Y.W.

Yu,^c Chun-Sing Lee*^b and Jun Xu*^a

^aSchool of Electronic Science & Applied Physics, Hefei University of Technology, Hefei 230009, P.

R. China

^bCenter of Super-Diamond and Advanced Films (COSDAF), and Department of Physics and

Materials Science, City University of Hong Kong, Hong Kong SAR, P. R. China

^cCenter of Super-Diamond and Advanced Films (COSDAF), and School of Energy and Environment,

City University of Hong Kong, Hong Kong SAR, P. R. China

^dState Key Laboratory of Heavy Oil Processing, and College of Science, China University of Petroleum (East China), Qingdao 266580, P. R. China

^ePhysics Laboratory, Industrial Training Center, Shenzhen Polytechnic, Shenzhen 518055, P. R. China

*Corresponding authors: apjunxu@hfut.edu.cn (J. Xu), apcslee@cityu.edu.hk (C.-S. Lee)



Fig. S1 TEM image and EDX mappings of the 2H-MoS $_{2x}$ Se $_{2-2x}$ nanospheres.



Fig. S2 I-V curves of the films of the three samples deposited on SiO_2 substrates, showing significant improvement in conductivity by post sulfuration treatment.



Fig. S3 (a) Nyquist plots of three electrodes after 3 cycles at the current density of 500 mA g⁻¹; (b) the relationship between Z' and $\omega^{-1/2}$ at low frequency.

The sodium ion diffusion coefficient (D) is calculated according to the following equation:

$$D = \frac{(RT)^2}{2(An^2F^2C\sigma)^2} \tag{1}$$

where *R* is the gas constant, *T* is the absolute temperature, *A* is the surface area of the electrode, *n* is the number of electrons per molecule during reduction, *F* is the Faraday constant, *C* is the molar concentration of sodium ions, and σ is the Warburg factor which has a relationship with *Z*':

$$Z' = R_s + R_{ct} + \sigma \omega^{-1/2} \tag{2}$$

The $Z'-\omega^{-1/2}$ plots of the three samples are presented in Fig. S3b. The σ value is estimated to be 245.9 $\Omega s^{1/2}$ for the freshly-prepared 1T-MoSe₂, 277.5 $\Omega s^{1/2}$ for the annealed 2H-MoSe₂, and 96.5 $\Omega s^{1/2}$ for the S-doped 2H-MoSe₂. As a result, it is calculated that the *D* values of the 1T-MoSe₂, 2H-MoSe₂, and 2H-MoS_{2x}Se_{2-2x} samples are 3.54×10^{-19} , 2.79×10^{-19} , and 2.30×10^{-18} cm² s⁻¹, respectively. Thus, the 2H-MoS_{2x}Se_{2-2x} sample obtained after sulfuration shows the fastest sodium ion diffusion rate.