Journal Name

ARTICLE

Electronic Supplementary Information

Enhancement of Anisotropic Thermoelectric Performance of Tungsten Disulfide by Titanium Doping

Zhiwei Huang,[ad §] Tianmin Wu,[c §] Shuang Kong,[ad] Qing-Long Meng,[a] Wei Zhuang,[*be] Peng Jiang[*a] and Xinhe Bao[*a]

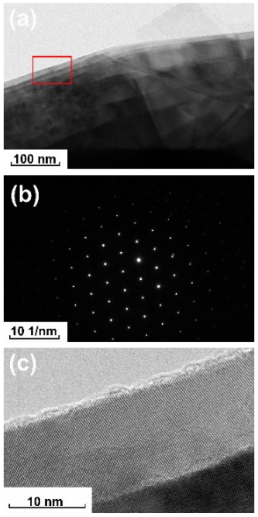

Fig. S1 (a) TEM image of $Ti_{0.1}WS_2$, (b) electron diffraction pattern of area marked by red rectangle in (a), (c) HRTEM image of area marked by red rectangle in (a).

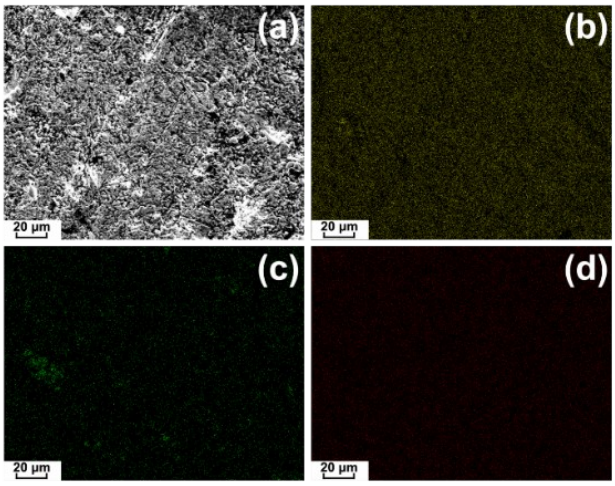

Fig. S2 (a) SEM image of polished $Ti_{0.1}WS_2$, (b-d) EDX elemental mapping of $Ti_{0.1}WS_2$, (b) Sulfur elemental mapping, (c) Titanium mapping, (d) Tungsten mapping.

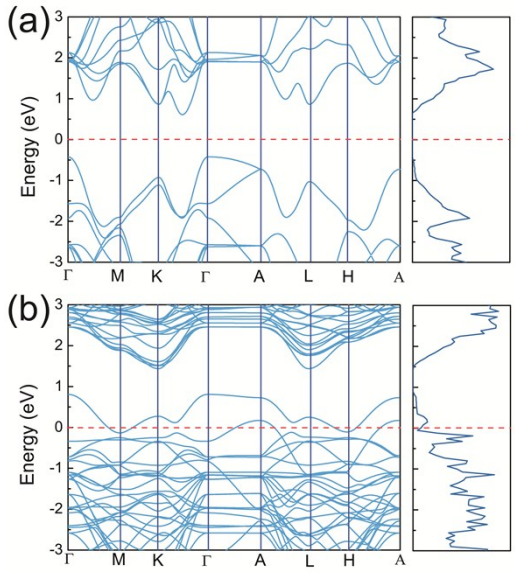

Fig. S3 Electronic band structure and DOS for (a) pristine WS_2, and (b) Ti doped WS_2 supercell.

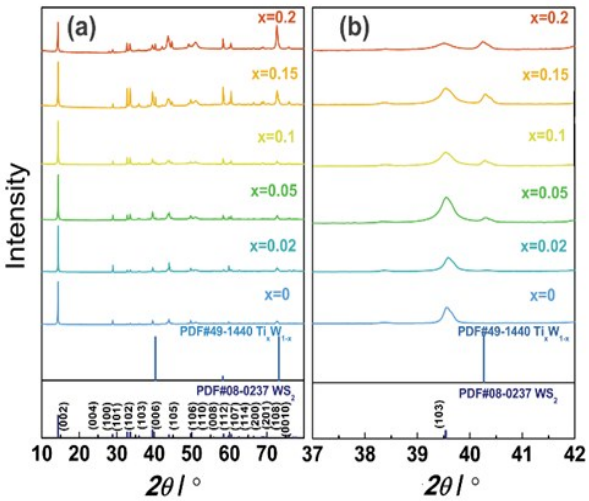

Fig. S4 (a) XRD pattern for Ti_xWS_2 (x=0, 0.02, 0.05, 0.1, 0.15, 0.20) along the direction perpendicular to pressing direction, (b) an enlarged view of XRD pattern around TiW alloy peak.

Calculation of Ti distribution

The distribution of Ti atoms in Ti_xWS_2 was calculated using XRD data. First, the mass ratio of TiW alloy (as second phase) was

calculated using relative intensity ratio (RIR) method.[19] The following equation was used:

$$W_B = \frac{I_B}{I_B + I_A K_A^B} \qquad (3)$$

where W_B is the mass ratio of TiW phase, I_B is the integrated intensity of the strongest peak of TiW phase, I_A is the integrated intensity of the strongest peak of WS_2 phase, K_A^B is the RIR ratio of two phases. Then the molar ratio of TiW/WS_2 (a) was calculated using $a=W_B*(xM_1+M_2)/M_3$, where x is the total molar ratio of Ti atoms in samples, M_1 is the molar mass of Ti atom, M_2 is the molar mass of WS_2, M_3 is the molar mass of TiW. The molar ratio of Ti atoms (b) in lattice was calculated using b=x-a, where x is the total molar ratio of Ti atoms.

x	**0.02**	**0.05**	**0.1**	**0.15**	**0.2**
a	0.006	0.012	0.015	0.023	0.026
b	0.014	0.038	0.085	0.127	0.174

Table. S1, Molar ratio of TiW phase (a) and Ti atoms in lattice (b).