Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary information

Identifying the effects of oxygen on the magnetism of WS_2 nanosheets

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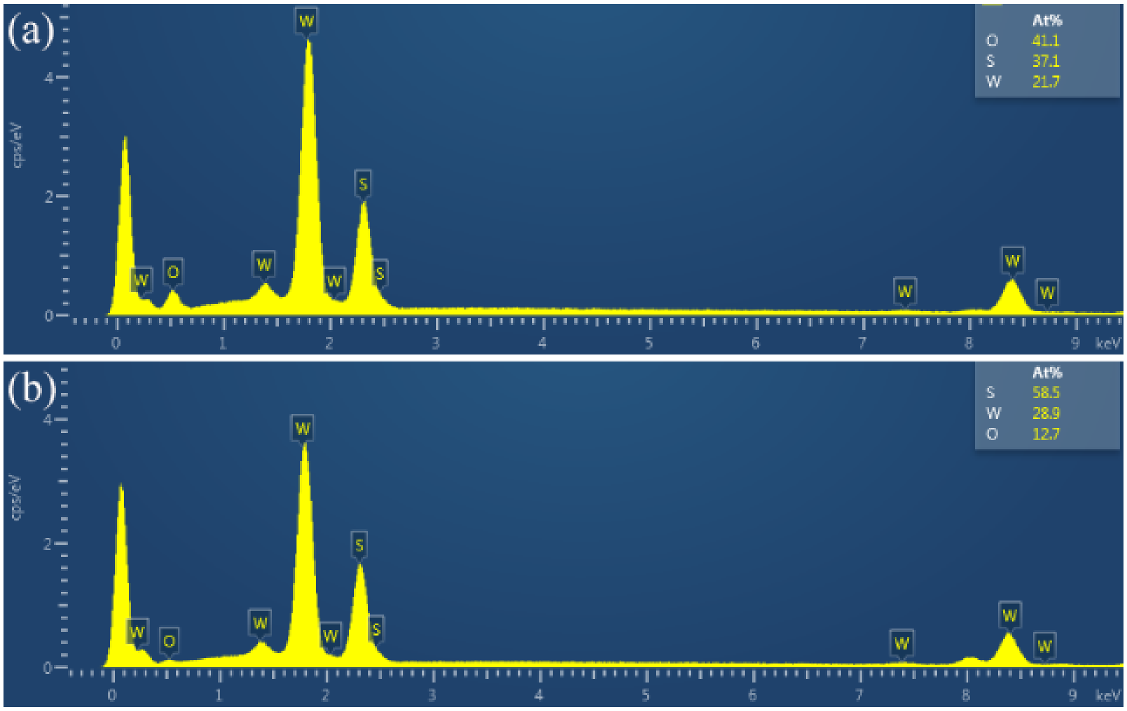

Fig. S1. (a) SEM-EDXS spectrum recorded on the exfoliated WS_2 nanosheets. (b) SEM-EDXS spectrum recorded on the sulfurized WS_2 nanosheets.

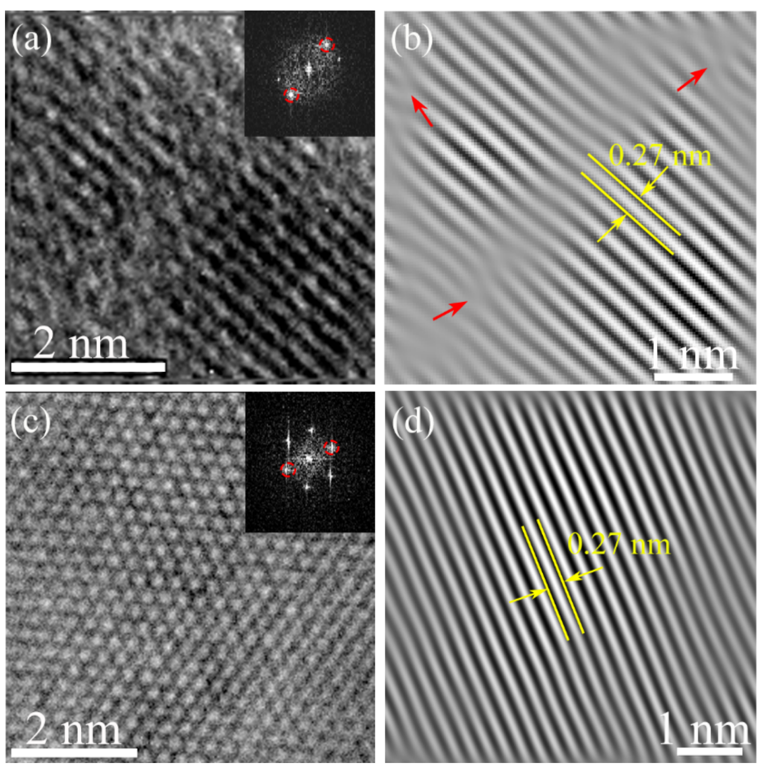

Fig. S2. (a) HRTEM image of the exfoliated WS_2 nanosheets and the corresponding FFT (inset). (b) the IFFT calculated from the FFT spots in the inset of panel (a). (c) HRTEM image of the sulfurized WS_2 nanosheets and the corresponding FFT (inset). (d) IFFT calculated from the FFT spots in the inset of panel (c).

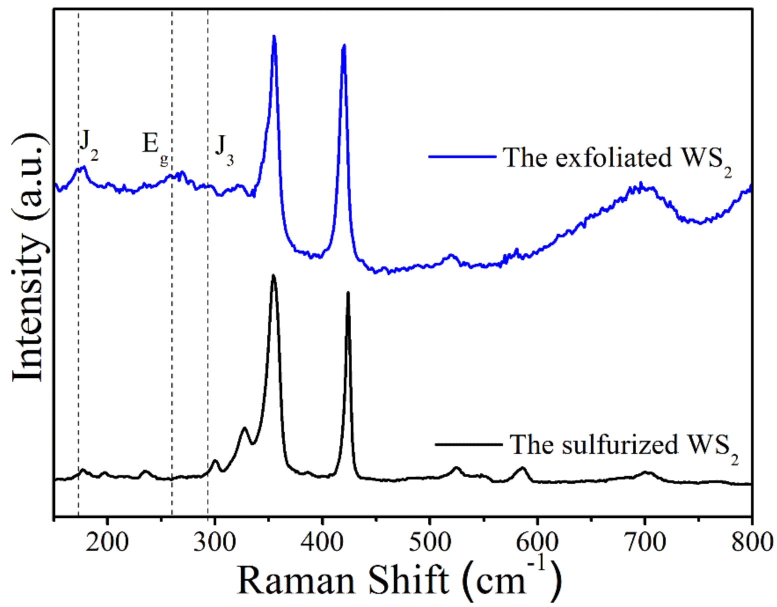

Fig. S3. The Raman spectra of the exfoliated and sulfurized WS_2 nanosheets.

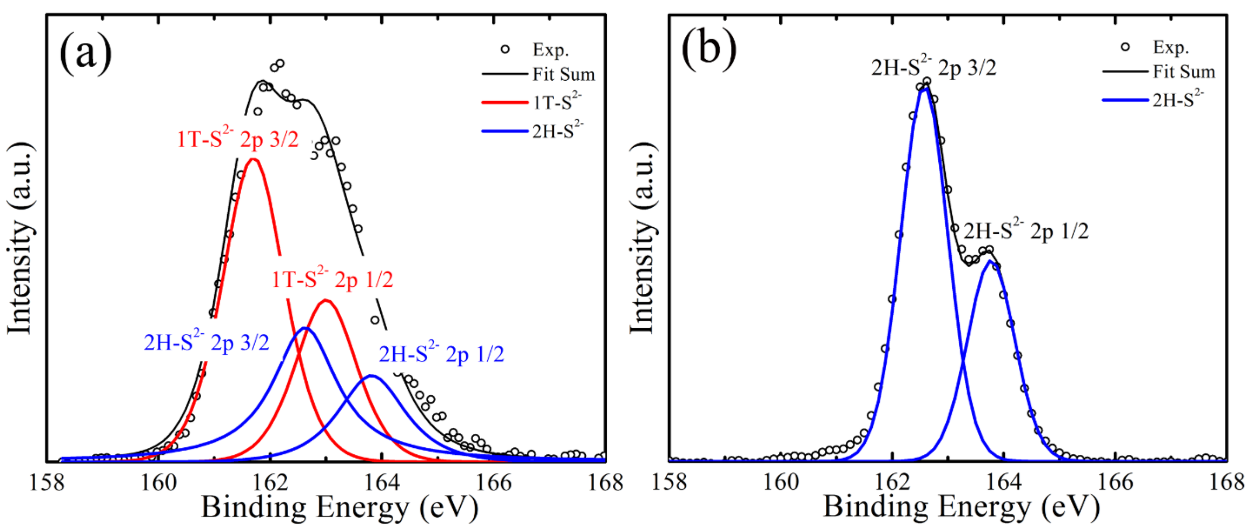

Fig. S4. (a) The typical fine-scanned S 2p spectrum of the exfoliated WS_2 nanosheets. The sub-peaks of 1T-S^{2-} and 2H-S^{2-} are denoted by red and blue lines, respectively. (b) The typical fine-scanned S 2p spectrum of the sulfurized WS_2 nanosheets.

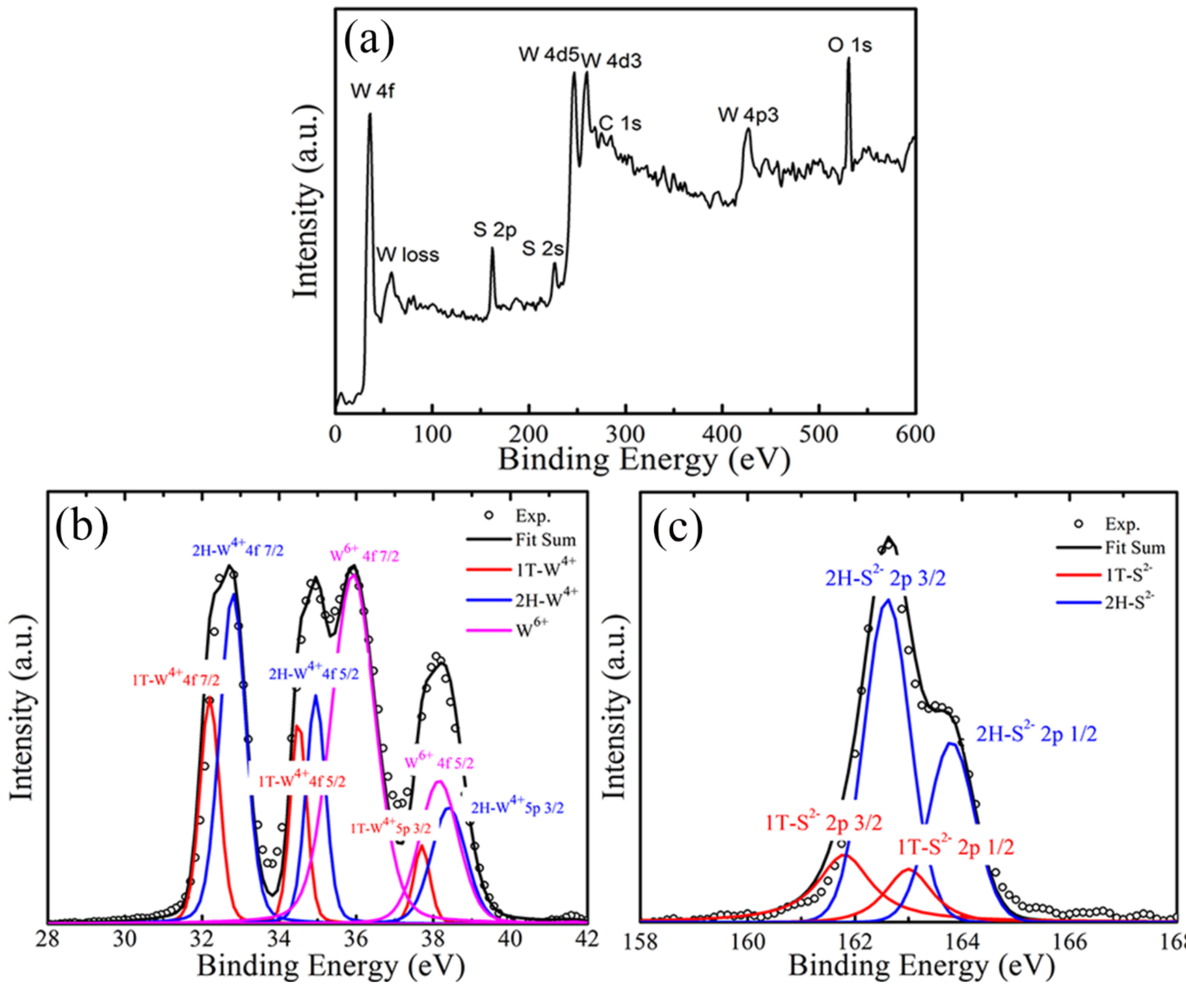

Fig. S5. (a) The XPS survey spectrum of the annealed WS_2 nanosheets. (b) The typical fine-scanned W 4f and 5p spectrum of the annealed WS2 nanosheets. The sub-peaks of 1T-W^{4+}, 2H-W^{4+} and W^{6+} are denoted by red, blue and magenta lines, respectively. (c) The typical fine-scanned S 2p spectrum of the annealed WS_2 nanosheets. The sub-peaks of 1T-S^{2-} and 2H-S^{2-} are denoted by red and blue lines, respectively.

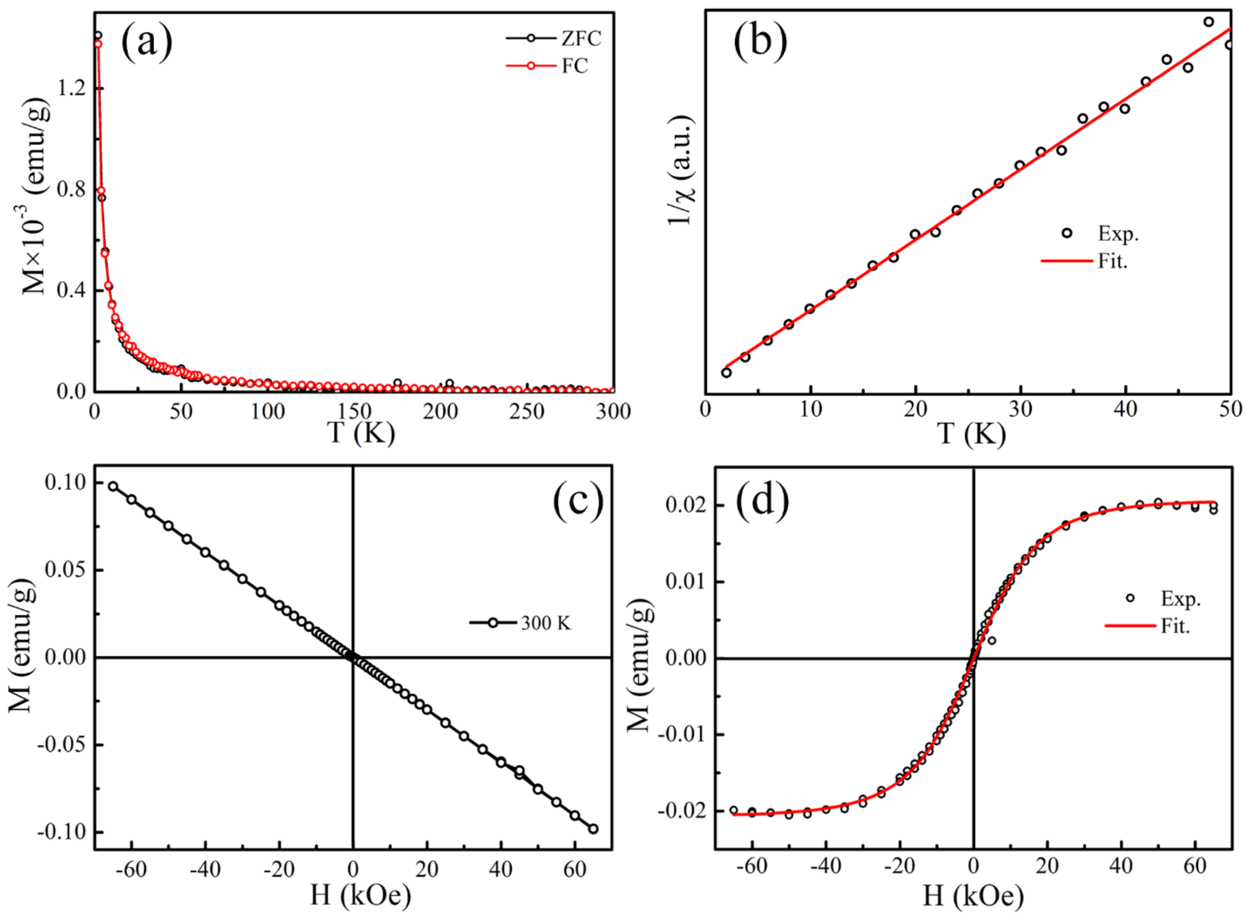

Fig. S6. The magnetic properties of the annealed WS_2 nanosheets. (a) ZFC and FC curves measured from 2 to 300 K under the applied field of 1 kOe. (b) $1/\chi - T$ curve measured from 2 to 50 K. The black symbols are the measurements and the red line is fitted by the Curie law. (c) The *M*–*H* curve measured at 300 K. (d) The *M*–*H* curve measured at 2 K. The black symbols are the measurements and the red line is fitted by the Brillouin function.

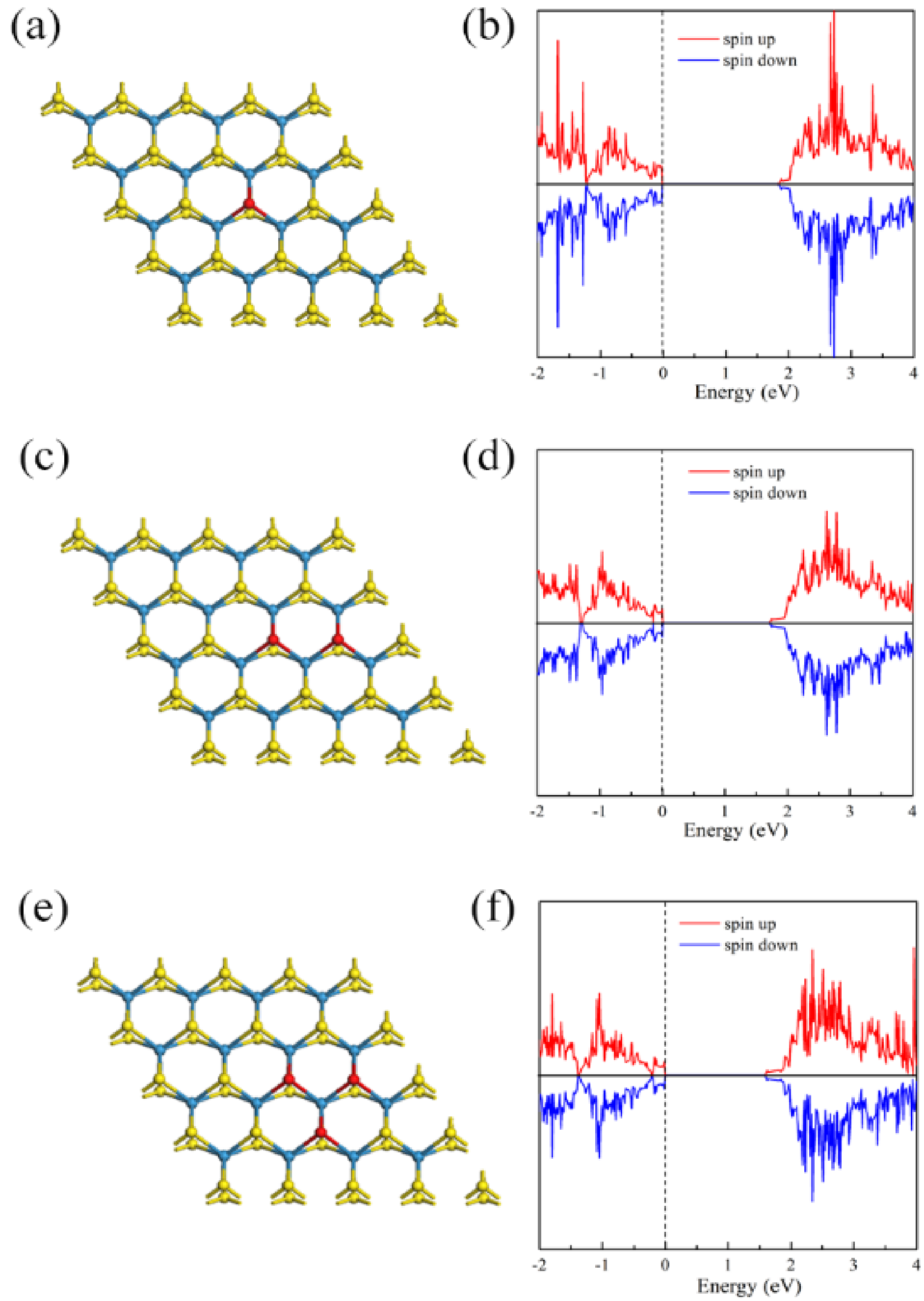

Fig. S7. (a) The structure and (b) the spin-polarized total DOS of WS_2 nanosheets with one sulfur atom substituded by oxygen. (c) The structure and (d) the spin-polarized total DOS of WS_2 nanosheets with two sulfur atoms substituded by oxygen. (e) The structure and (f) the spin-polarized total DOS of WS_2 nanosheets with three sulfur atoms substituded by oxygen.

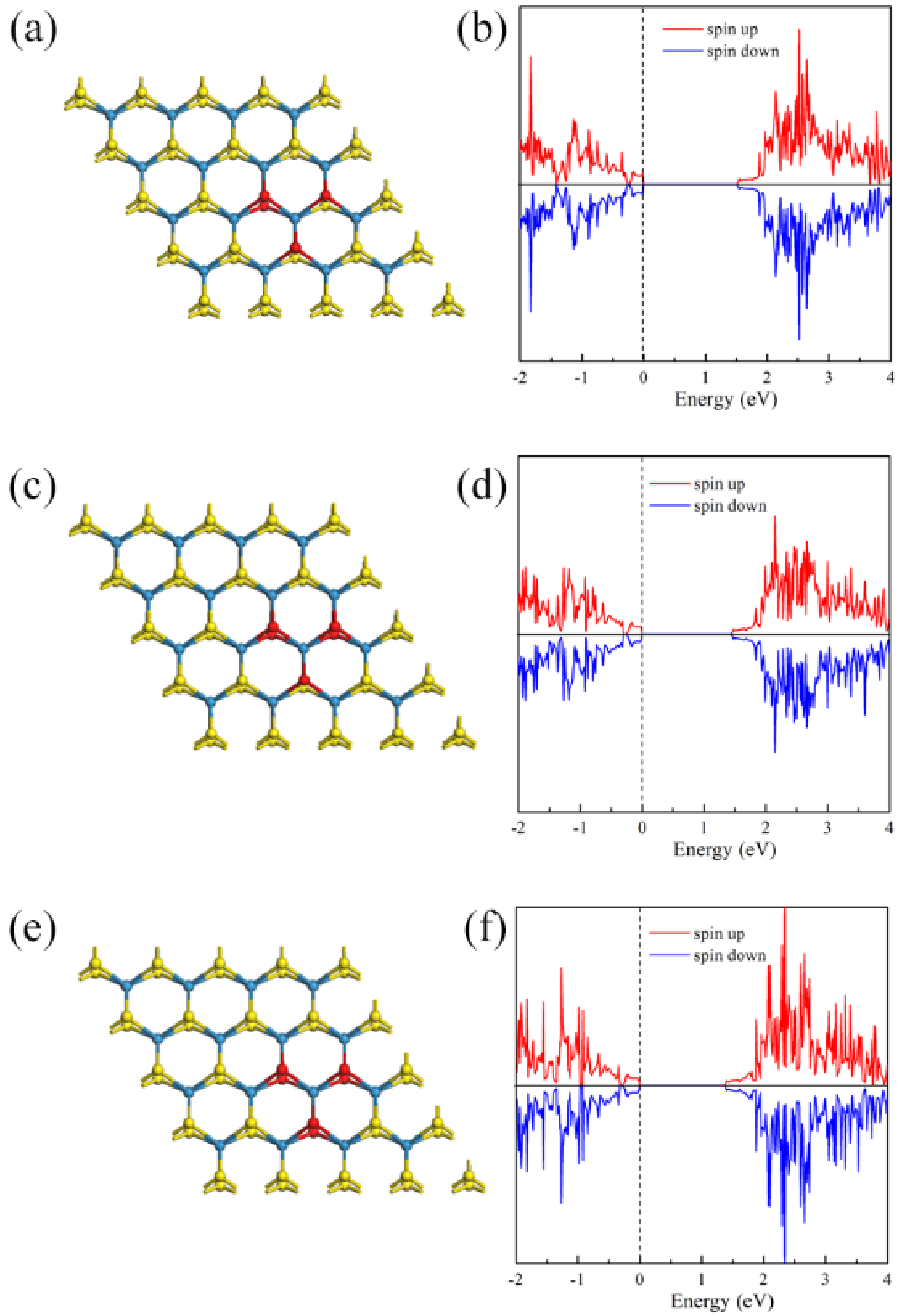

Fig. S8. (a) The structure and (b) the spin-polarized total DOS of WS_2 nanosheets with four sulfur atoms substituded by oxygen. (c) The structure and (d) the spin-polarized total DOS of WS_2 nanosheets with five sulfur atoms substituded by oxygen. (e) The structure and (f) the spin-polarized total DOS of WS_2 nanosheets with six sulfur atoms substituded by oxygen.

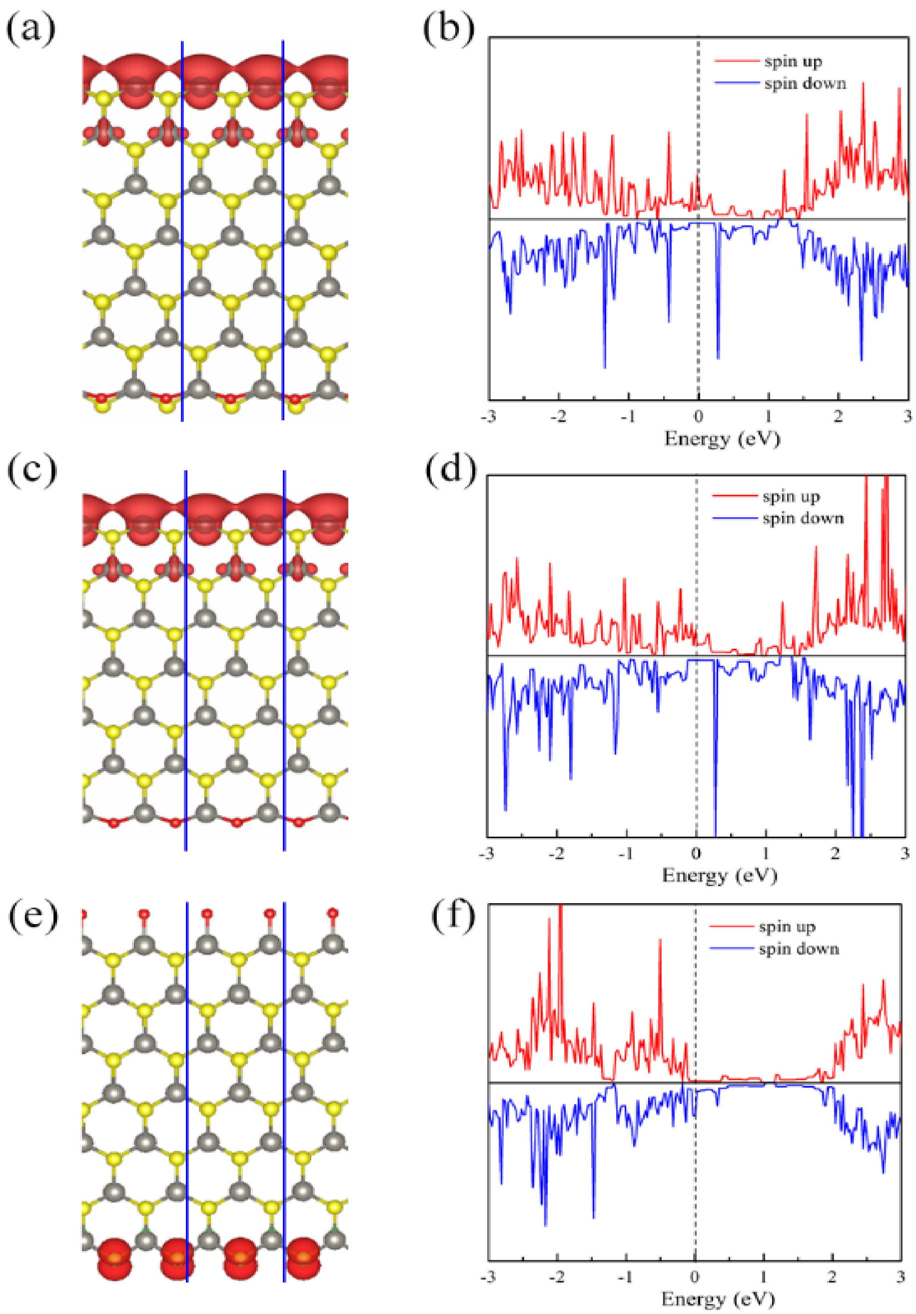

Fig. S9. (a) the net spin density distribution and (b) the spin-polarized DOS of WS_2-ZNRs with one S atom at the edge substitued by oxygen (WS_2-ZNRs-1Os). (c) the net spin density distribution and (d) the spin-polarized DOS of WS_2-ZNRs with two S atoms at the edge substitued by oxygen (WS_2-ZNRs-2Os). (e) the net spin density distribution and (f) the spin-polarized DOS of WS_2-ZNRs with the edge W atoms bonding with oxygen (WS_2-ZNRs-1$O_{ad\text{-}W}$). The unit cells are depicted by the blue lines.

Table S1 The magnetic moments (μ_B) of the unit cells for the single-layer WS_2 with sulfur atoms substituted by oxygen.

sample	$1O_S$	$2O_S$	$3O_S$	$4O_S$	$5O_S$	$6O_S$
M (μ_B)	0.001	0	0.003	0.003	0.003	0