Electronic Supplementary Information for

Synergistic vacancy defect and mechanical strain for the mechanical, electronic and optical properties modulation of monolayer tungsten disulfide

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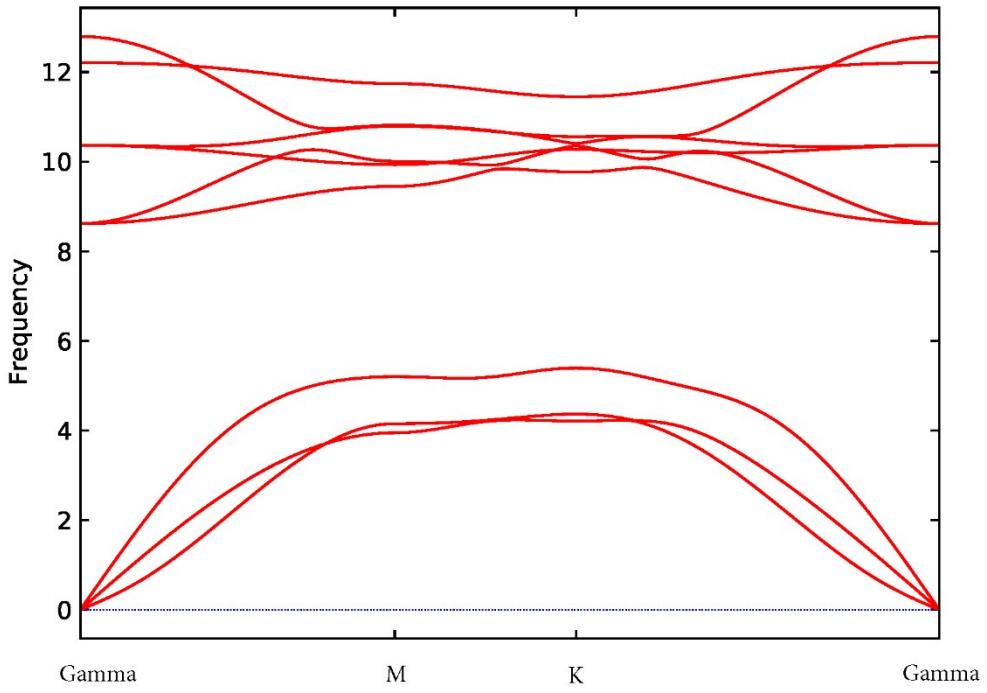

Figure S1. The phonon spectrum of pristine monolayer WS2.

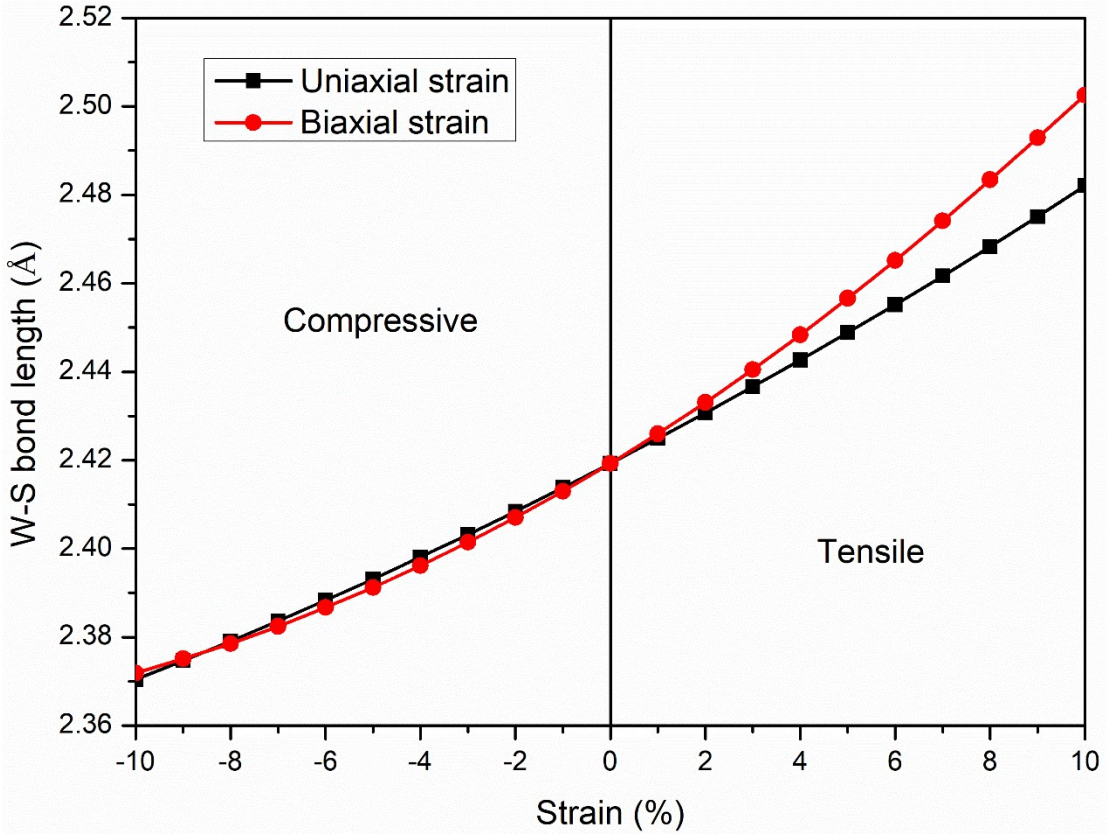

Figure S2. Variation of W-S bond length of pristine monolayer WS2 with applied

strain.

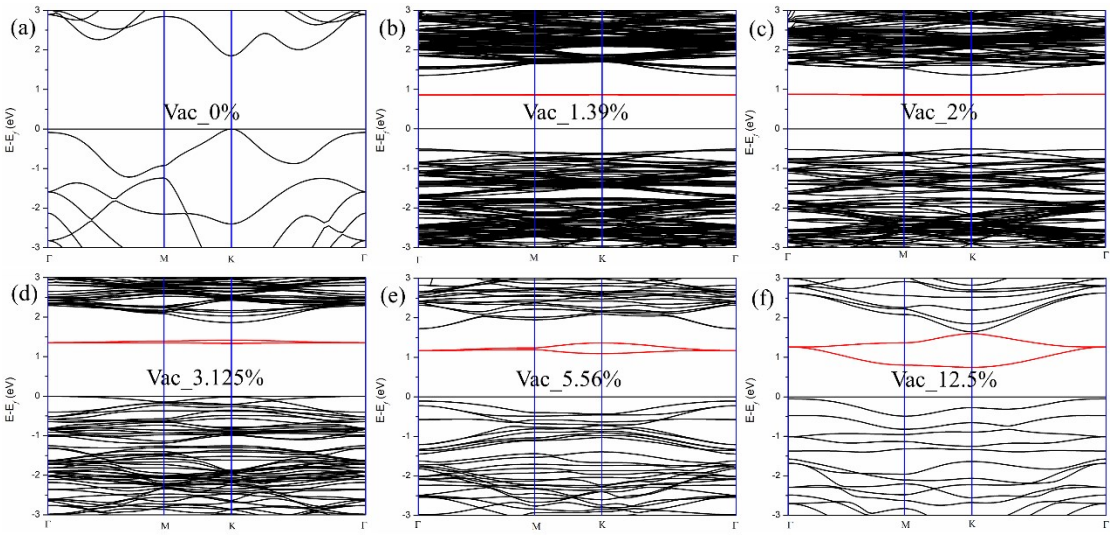

Figure S3. Electronic band structure of unstrained monolayer WS_2 with different sulfur vacancy concentrations of (a) 0%, (b) 1.39%, (c) 2%, (d) 3.125%, (e) 5.56%, and (f) 12.5%, respectively. The defective states are highlighted with red lines, and the horizontal solid line indicates the Fermi level, which is set to 0 eV.

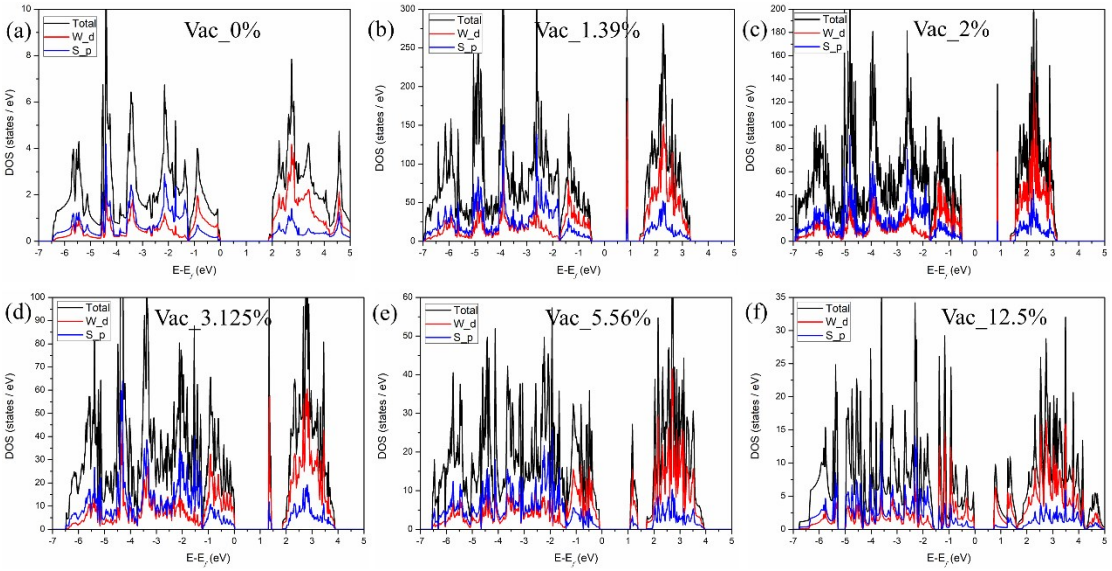

Figure S4. Electronic total (TDOS) and partial density of states (PDOS) of unstrained monolayer WS_2 with different sulfur vacancy concentrations of (a) 0%, (b) 1.39%, (c) 2%, (d) 3.125%, (e) 5.56%, and (f) 12.5%, respectively.

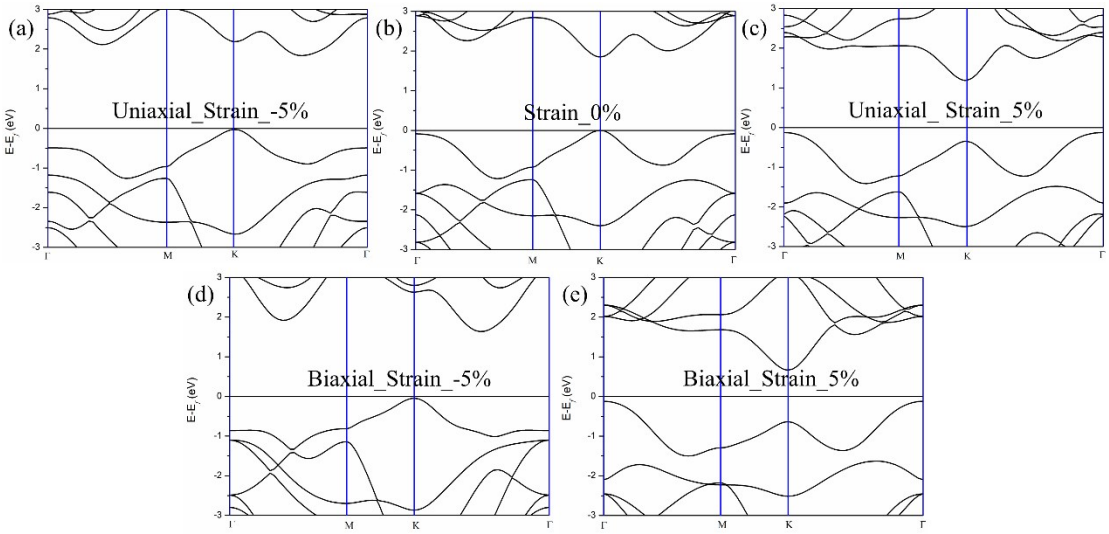

Figure S5. Electronic band structure of the pristine monolayer WS_2 under different applied strains of (a) -5% uniaxial strain, (b) strain-free, (c) 5% uniaxial strain, (d) -5% biaxial strain and (e) 5% biaxial strain, respectively. The horizontal solid line indicates the Fermi level, which is set to 0 eV.

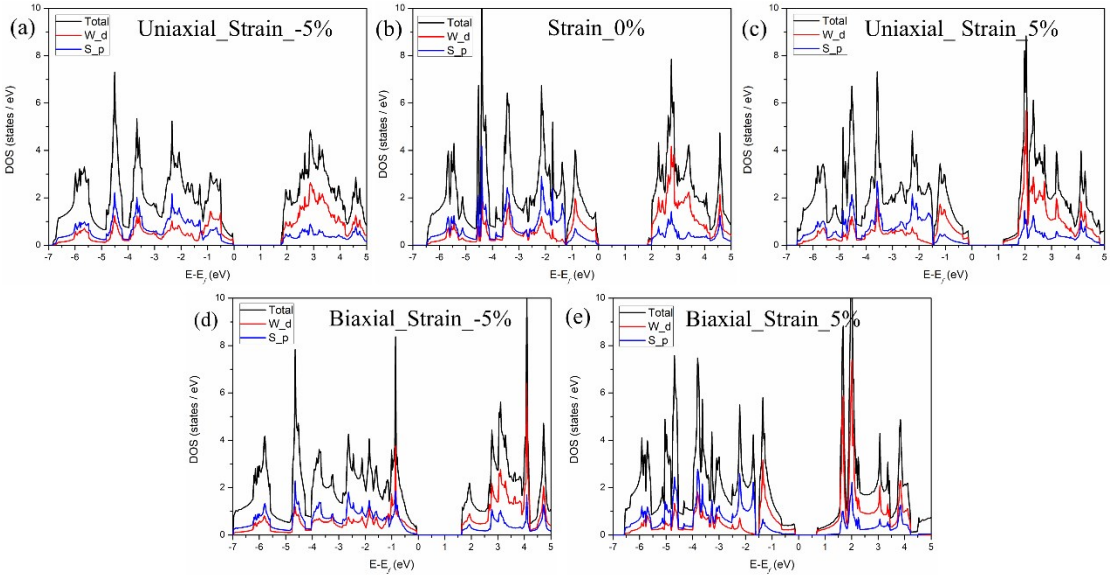

Figure S6. Electronic TDOS and PDOS of the pristine monolayer WS_2 under different applied strains of (a) -5% uniaxial strain, (b) strain-free, (c) 5% uniaxial strain, (d) -5% biaxial strain and (e) 5% biaxial strain, respectively.

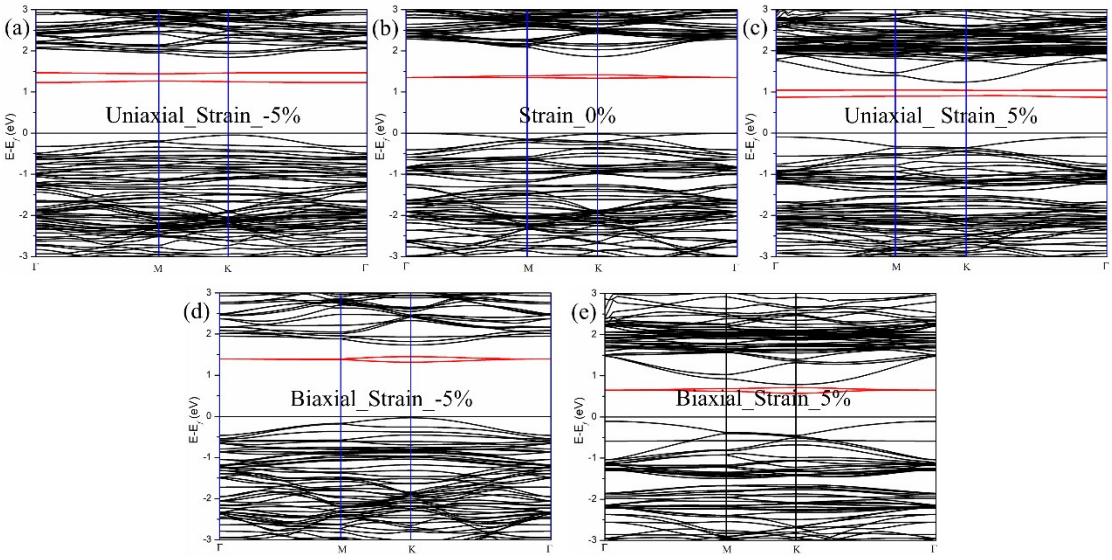

Figure S7. Electronic band structure of monolayer WS_2 with sulfur vacancy concentration of 3.125% under different applied strains of (a) -5% uniaxial strain, (b) strain-free, (c) 5% uniaxial strain, (d) -5% biaxial strain and (e) 5% biaxial strain, respectively. The defective states are highlighted with red lines, and the horizontal solid line indicates the Fermi level, which is set to 0 eV.

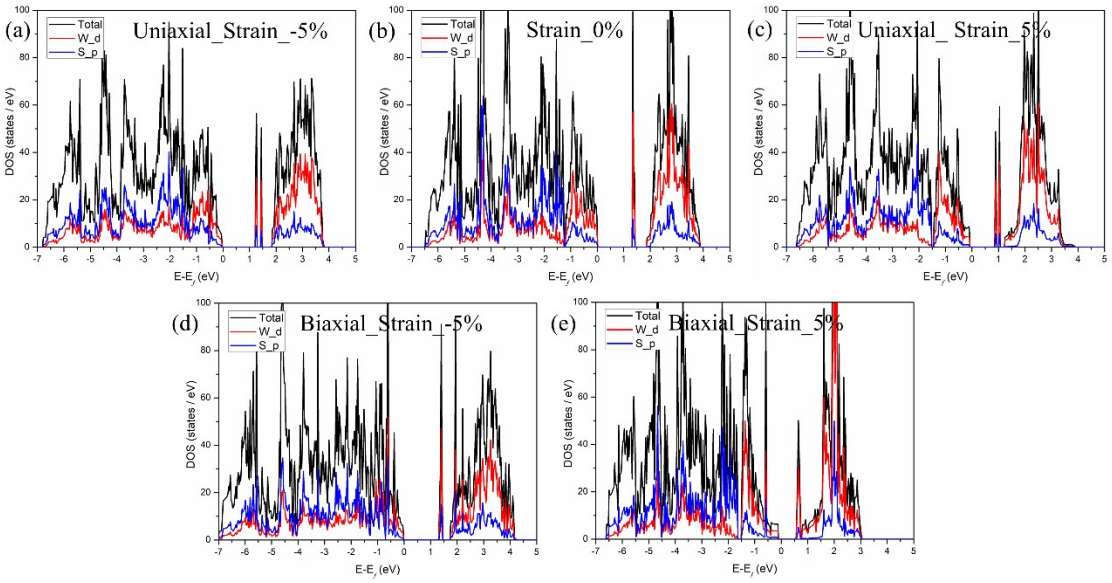

Figure S8. Electronic TDOS and PDOS of monolayer WS_2 with sulfur vacancy concentration of 3.125% under different applied strains of (a) -5% uniaxial strain, (b) strain-free, (c) 5% uniaxial strain, (d) -5% biaxial strain and (e) 5% biaxial strain, respectively.