Supporting information

A comprehensive study on the effects of gamma radiation on the physical properties of two-dimensional WS_2 monolayer semiconductor

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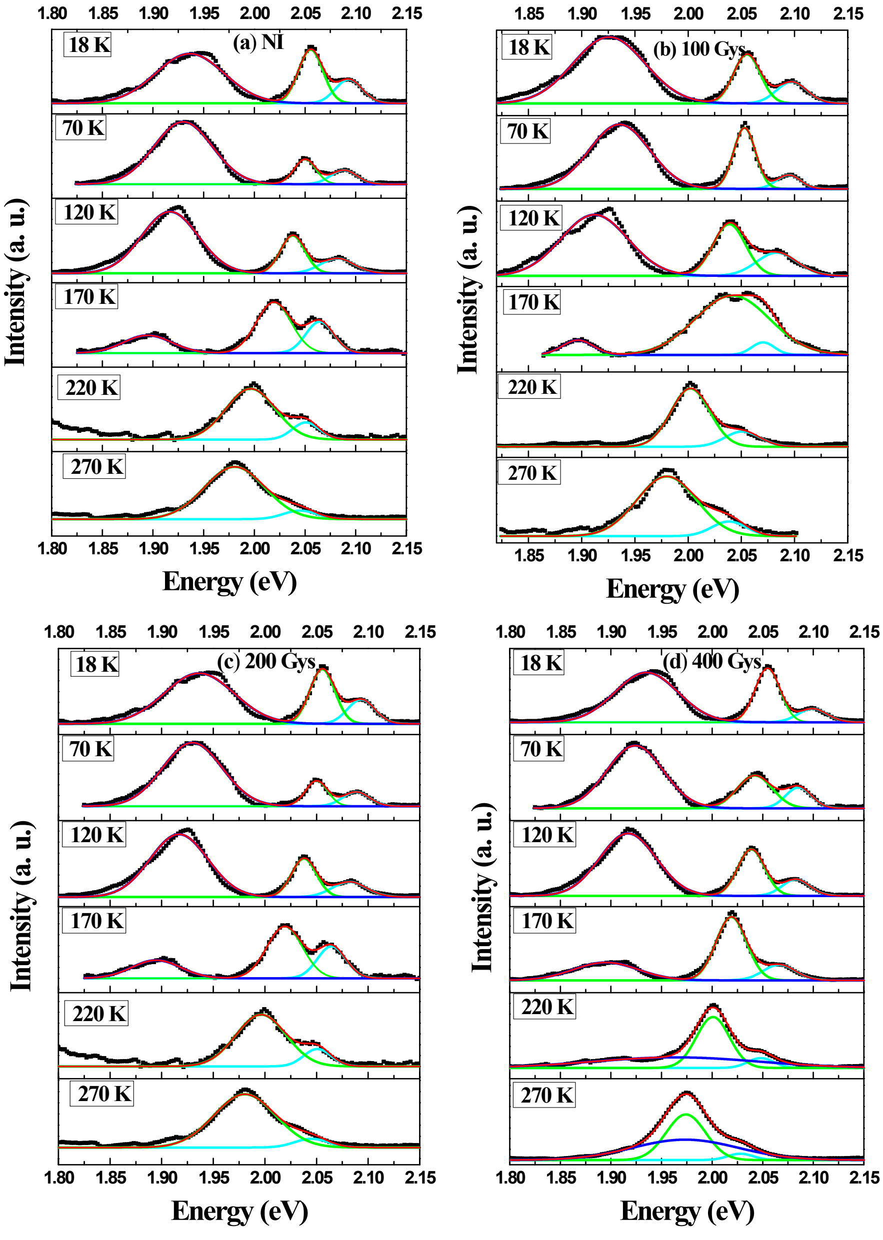


Fig. S1 PL spectra at different temperatures as a function of irradiation dose and their respective peak deconvolution. (a) Non-radiated (NI) sample, and radiated samples (b) 100 Gys, (c) 200 Gys, (d) 400 Gys.

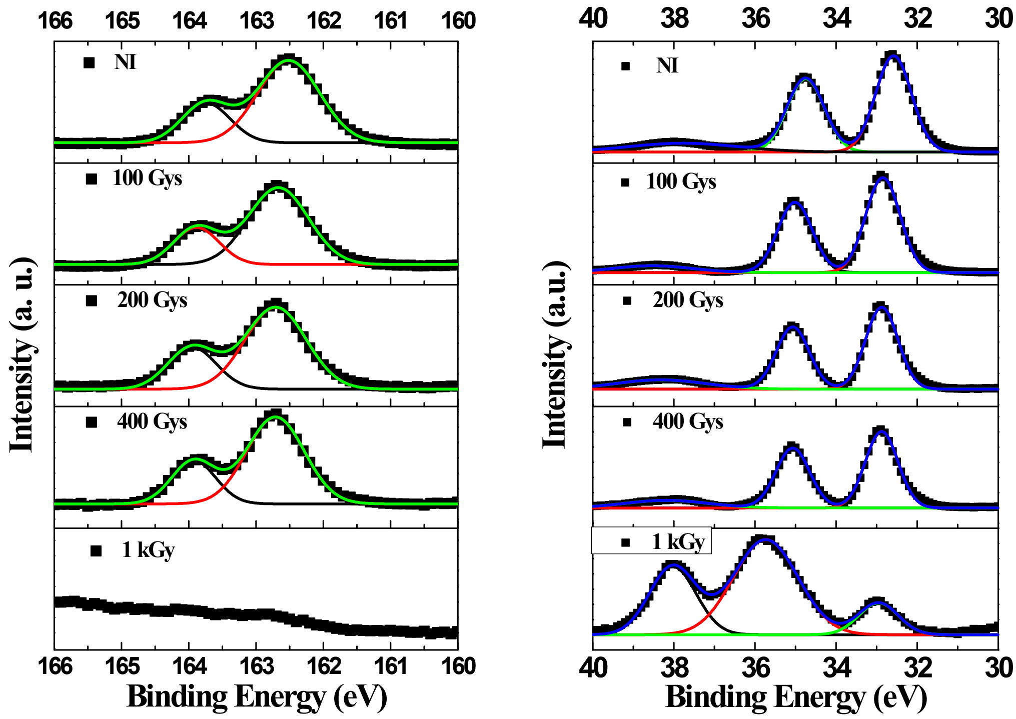


Fig. S2 XPS spectrum of the Non-irradiated (NI) and irradiated samples, all showing two and three peaks for the S2p and W4f core levels, respectively, as reported previously for 2D-WS_2. The solid lines represent their respective peak deconvolution.

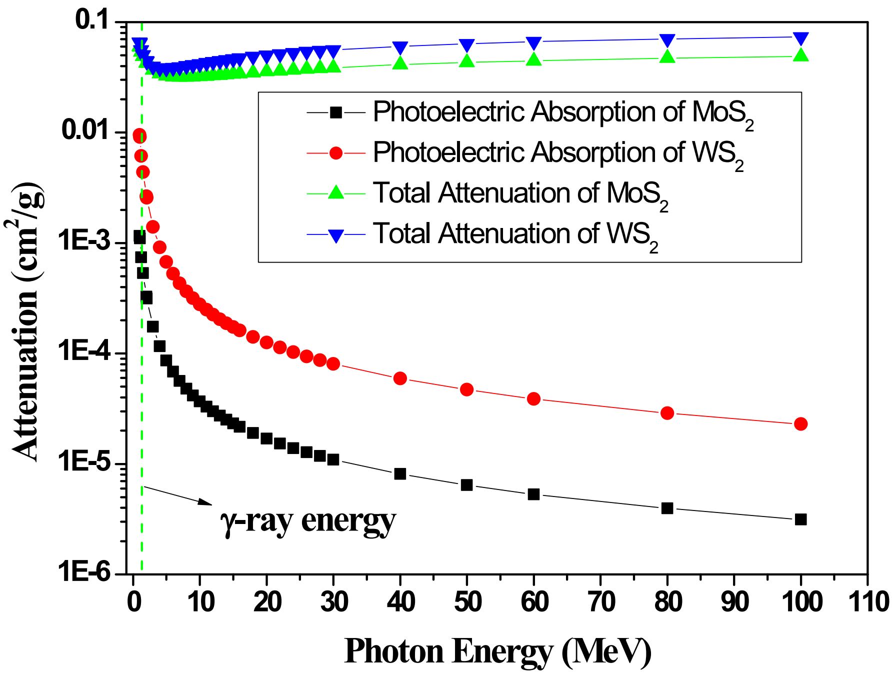
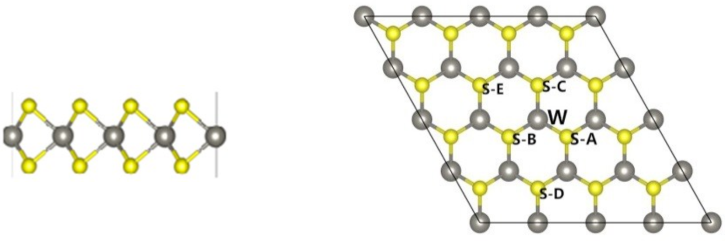


Fig. S3 XCOM plots showing the γ -ray scattering mechanisms in MoS_2 and WS_2 as a function of radiation energies. The average energy for the Co^{60} γ –rays, which is around 1.33 MeV is also shown as a reference.

The following figures show the schematic crystal structures of a perfect WS_2 monolayer (Fig. S4) and defective one with V_{1W+2S} vacancies composed of one tungsten and a pair of its nearby sulfurs (Fig.S5), which were used in the DFT calculations.



(a) (b)

Fig. S4 Side (a) and top (b) views of perfect WS_2 monolayer. The gray and yellow spheres represent W and S atoms, respectively. The letters W, S-A, S-B,…, and S-E label W atom and its five neighbor S atoms.

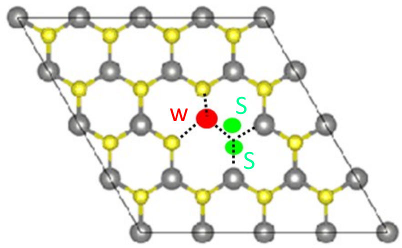


Fig. S5 WS_2 monolayer with V_{1W+2S} vacancy complex, consisting of one W vacancy (red sphere) and nearby one sulfur vacancy pair (green spheres) in upper and lower layers at A site. The gray and yellow spheres represent W and S atoms, respectively.Total magnetic moment is equal to 2.0 μB.

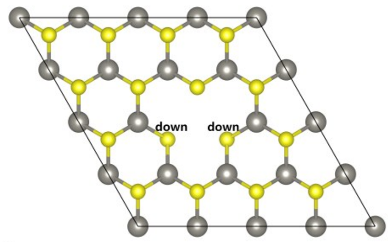


Fig. S6 V_{1W+2S} vacancy complex consisting of W, S-A_{up} and S-B_{up} vacancies with M_{tot}=0 μB.

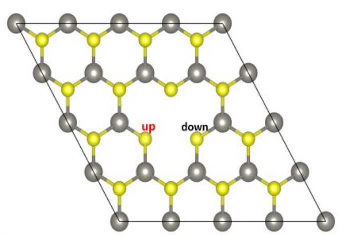


Fig. S7 V_{1W+2S} vacancy complex consisting of W, S-A_{up} and S-B_{down} vacancies with M_{tot}=0 μB.

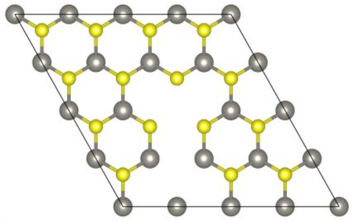


Fig. S8 V_{1W+2S} vacancy complex consisting of W, S-D_{up} and S-D_{down} vacancies with M_{tot}=0 μB.

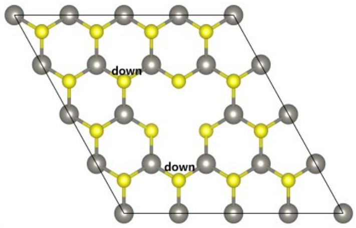


Fig. S9 V_{1W+2S} vacancy complex consisting of W, S-D_{up} and S-E_{up} vacancies with M_{tot}=0 μB.

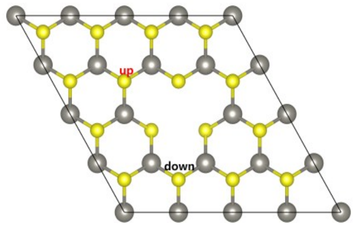


Fig. S9 V_{1W+2S} vacancy complex consisting of W, S-D_{up} and S-E_{down} vacancies with M_{tot}=0 μB.

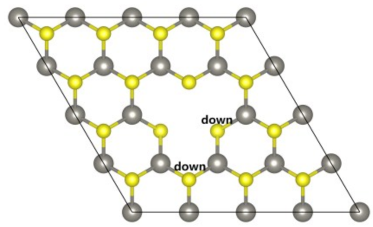


Fig. S10 V_{1W+2S} vacancy complex consisting of W, S-A_{up} and S-D_{up} vacancies with M_{tot}=0 μB.

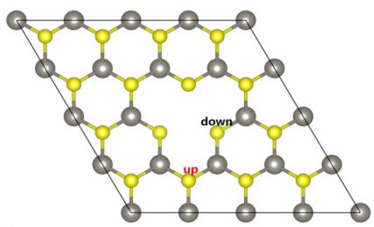


Fig. S11 V_{1W+2S} vacancy complex consisting of W, S-A_{up} and S-D_{down} vacancies with M_{tot}=0 μB.

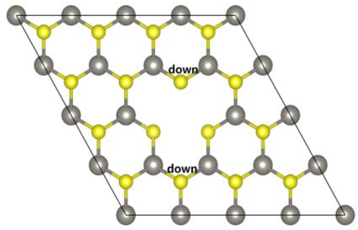


Fig. S12 V_{1W+2S} vacancy complex consisting of W, S-C_{up} and S-D_{up} vacancies with M_{tot}=0 μB.

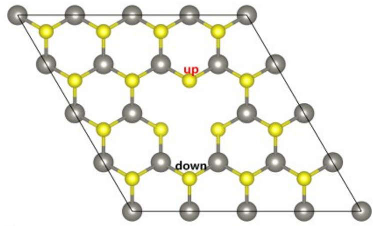


Fig. S13 V_{1W+2S} vacancy complex consisting of W, S-C_{down} and S-D_{up} vacancies with M_{tot}=0 μB.