SUPPLEMENTARY INFORMATION:

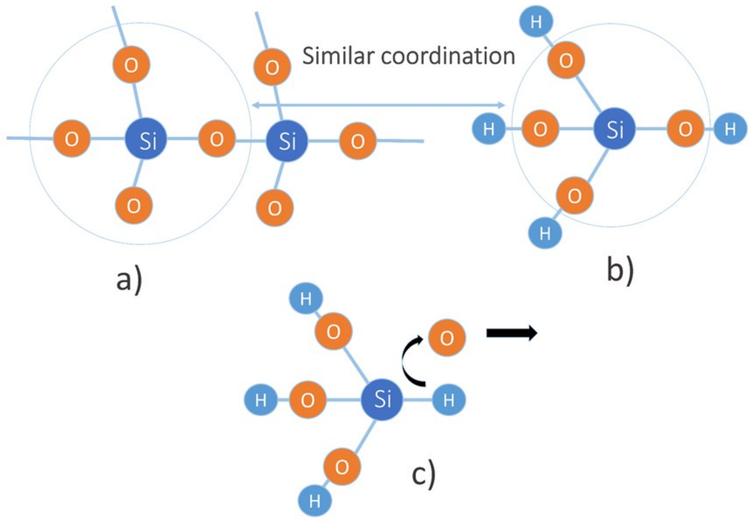

Figure S1: The reaction with bulk oxides and surface oxide groups (-OH) are performed using a similar coordination molecule. a) A normal SiO_2 coordination pattern. b) A free standing molecule with the same coordination for the oxygen donating species as that in pure SiO_2. c) The molecule in b) donates an oxygen for reaction.

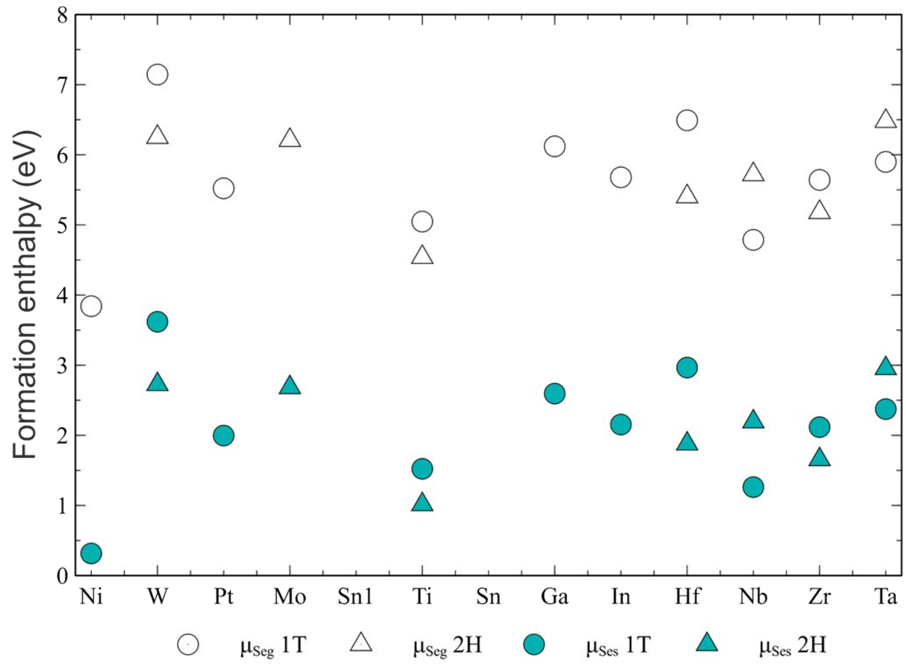

Figure S2: ΔH_{Sev} (formation energy of Selenium vacancies) assuming the release of Se in gas and in a solid phase is shown on the vertical axis. The horizontal axis shows the coordinating cation used in MX_2 . Whenever identified, the impact of different phases of the 2D material(1T/2H) is listed for a particular metal. Not every phase exists for every cation. Open and closed symbols correspond to 1T and 2H phases respectively.

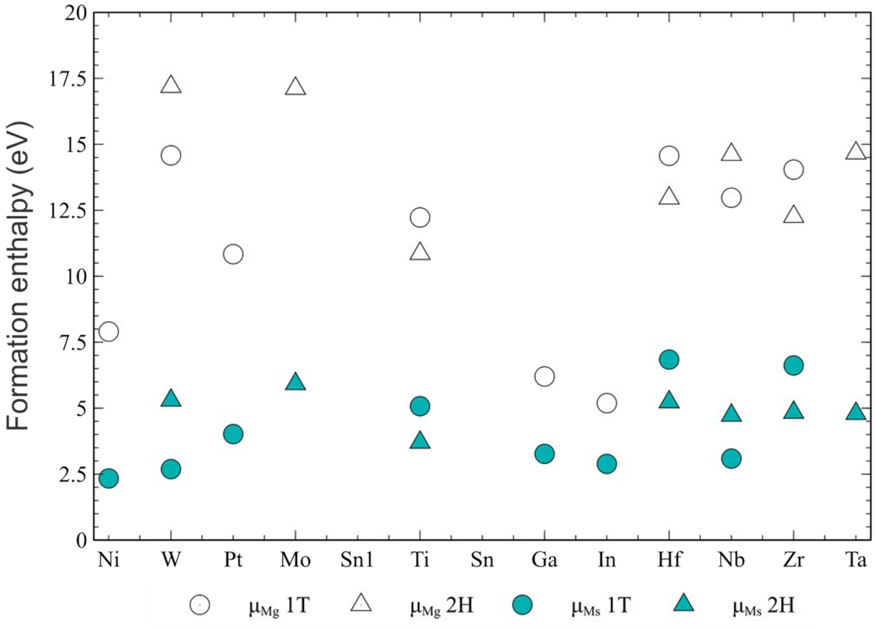

Figure S3: ΔH_{Mv} (formation energy of metal vacancies) in Selenides assuming the release of metal in gas and in a solid phase. The horizontal axis shows the coordinating cation used in MX_2 . Whenever identified, the impact of different phases of the 2D material(1T/2H) is listed for a particular metal. Note that not every metal has a corresponding phase of the 2D material. Open and closed symbols correspond to 1T and 2H phases respectively.

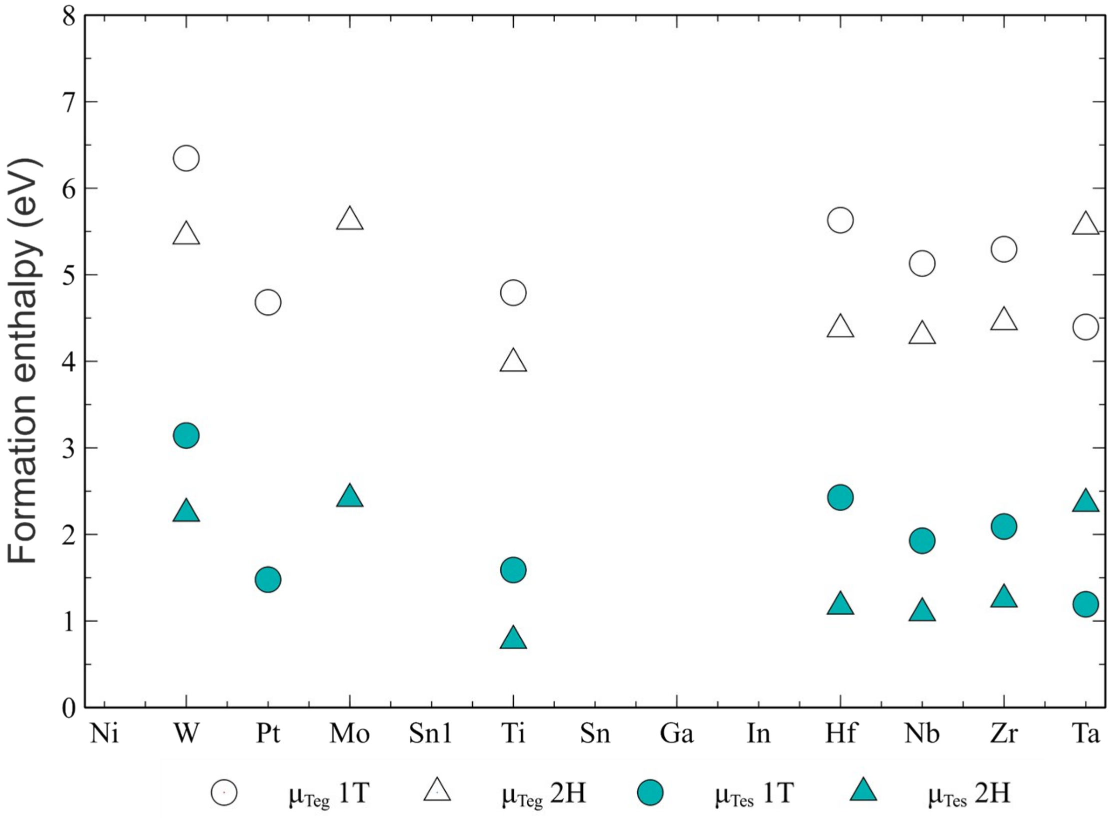

Figure S4: ΔH_{Tev} (formation energy of Tellurium vacancies) assuming the release of Te in gas and in a solid phase is shown on the vertical axis. The horizontal axis shows the coordinating cation used in MX_2 . Whenever identified, the impact of different phases of the 2D material(1T/2H) is listed for a particular metal. Note that not every metal has a corresponding phase of the 2D material. Circles and triangles correspond to 1T and 2H phases respectively.

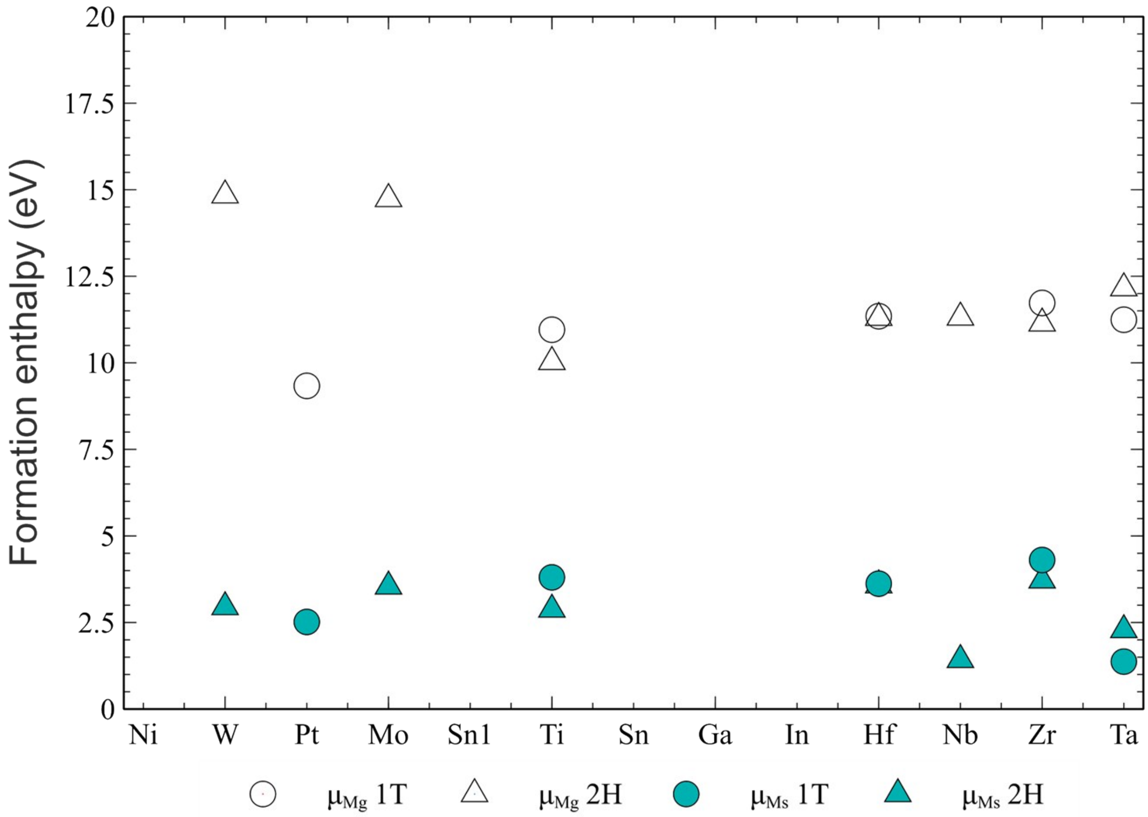

Figure S5: ΔH_{Mv} (formation energy of metal vacancies) in Tellurides assuming the release of metal in gas and in a solid phase. The horizontal axis shows the coordinating cation used in MX_2 . Whenever identified, the impact of different phases of the 2D material(1T/2H) is listed for a particular metal. Note that not every metal has a corresponding phase of the 2D material. Circles and triangles correspond to 1T and 2H phases respectively.

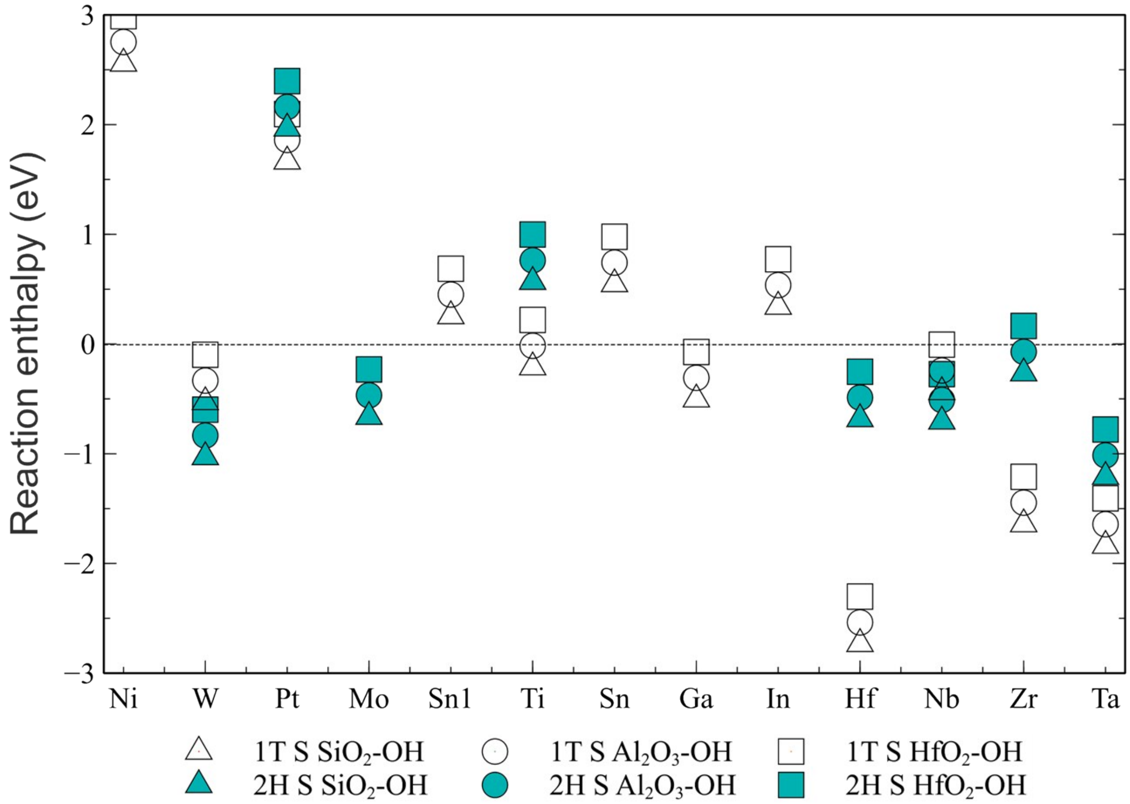

Figure S6: Reaction enthalpies for a sulfur vacancy and the surface hydroxyl groups of SiO2, Al2O3 and HfO2. The enthalpies suggest that surface hydroxyl groups in SiO2 are the most reactive. However, the difference in the three dielectric surface groups is not very large.

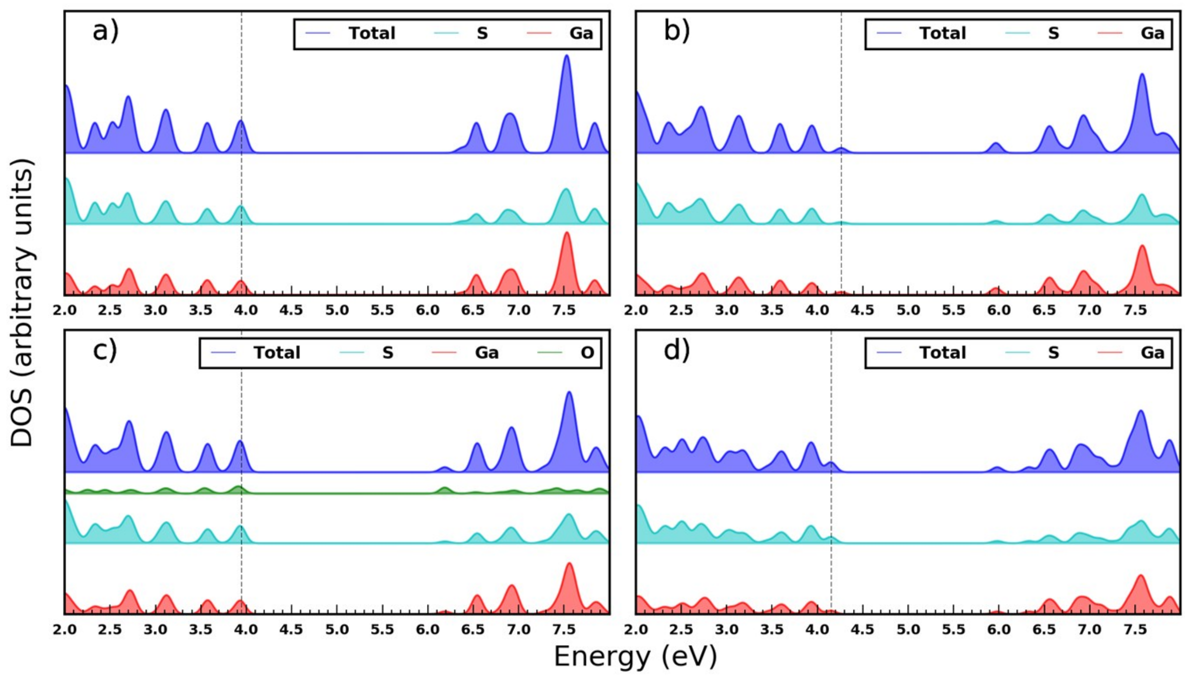

Figure S7: a) Shows the DOS for pristine GaS with individual contributions. b) Shows the dos for GaS with one sulfur vacancy. c) Shows the DOS with sulfur vacancy replaced by an oxygen atom. d) Shows the impact of an Ga vacancy on the DOS.

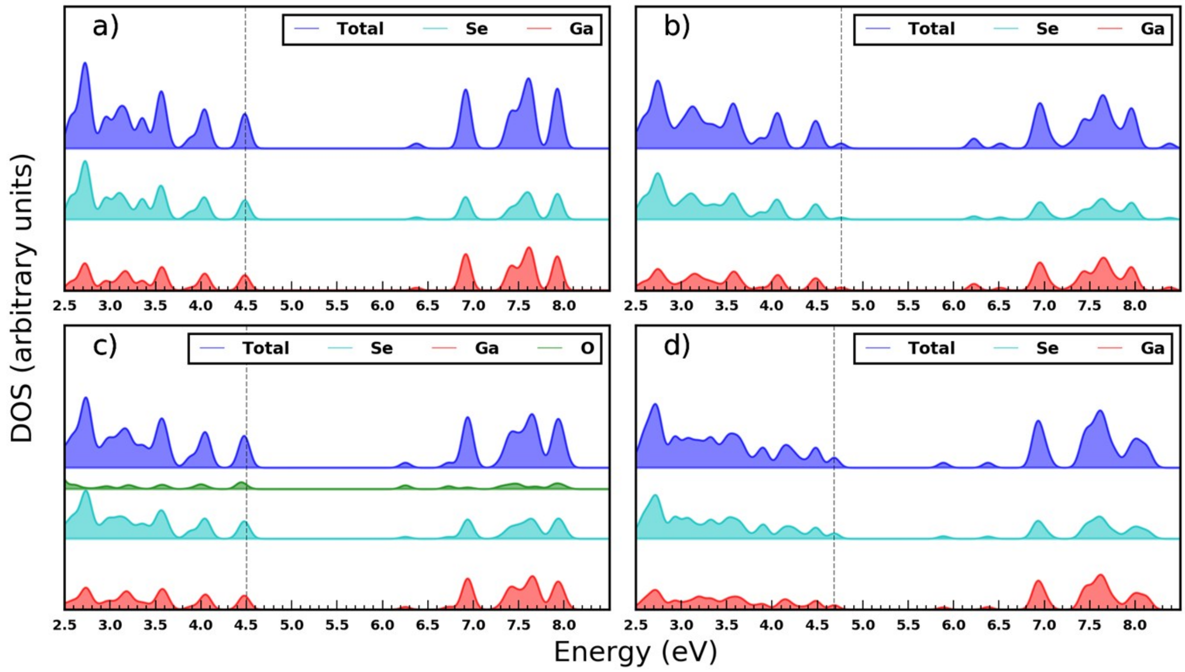

Figure S8: a) Shows the DOS for pristine GaSe with individual contributions. b) Shows the dos for GaSe with one Selenium vacancy. c) Shows the DOS with Selenium vacancy replaced by an oxygen atom. d) Shows the impact of an Ga vacancy on the DOS.

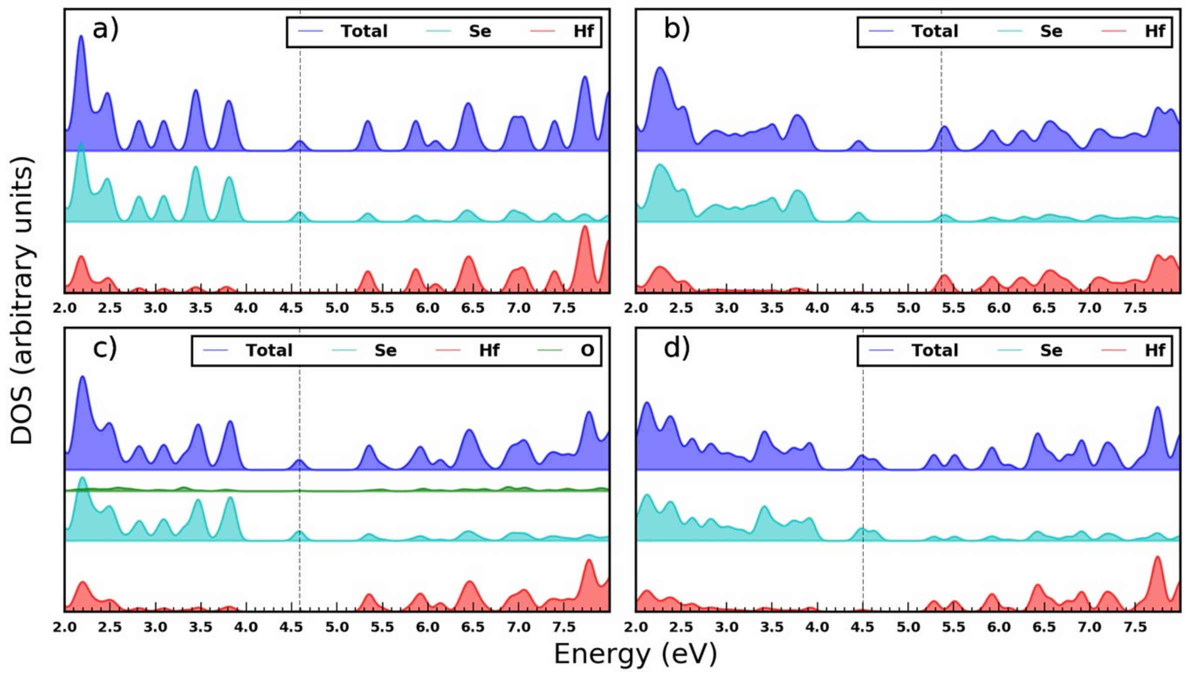

Figure S9: a) Shows the DOS for pristine $HfSe_2$-1T with individual contributions. b) Shows the dos for $HfSe_2$-1T with one Selenium vacancy. c) Shows the DOS with Selenium vacancy replaced by an oxygen atom. d) Shows the impact of an Hf vacancy on the DOS.

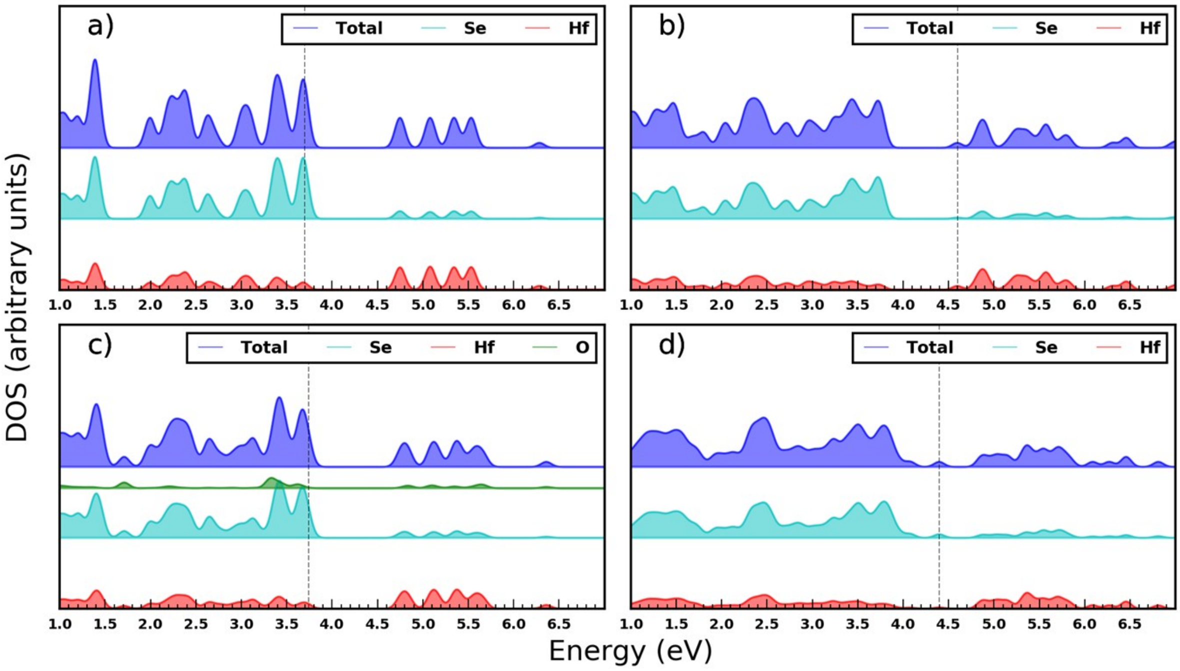

Figure S10: a) Shows the DOS for pristine $HfSe_2$-2H with individual contributions. b) Shows the dos for $HfSe_2$-2H with one Selenium vacancy. c) Shows the DOS with Selenium vacancy replaced by an oxygen atom. d) Shows the impact of an Hf vacancy on the DOS.

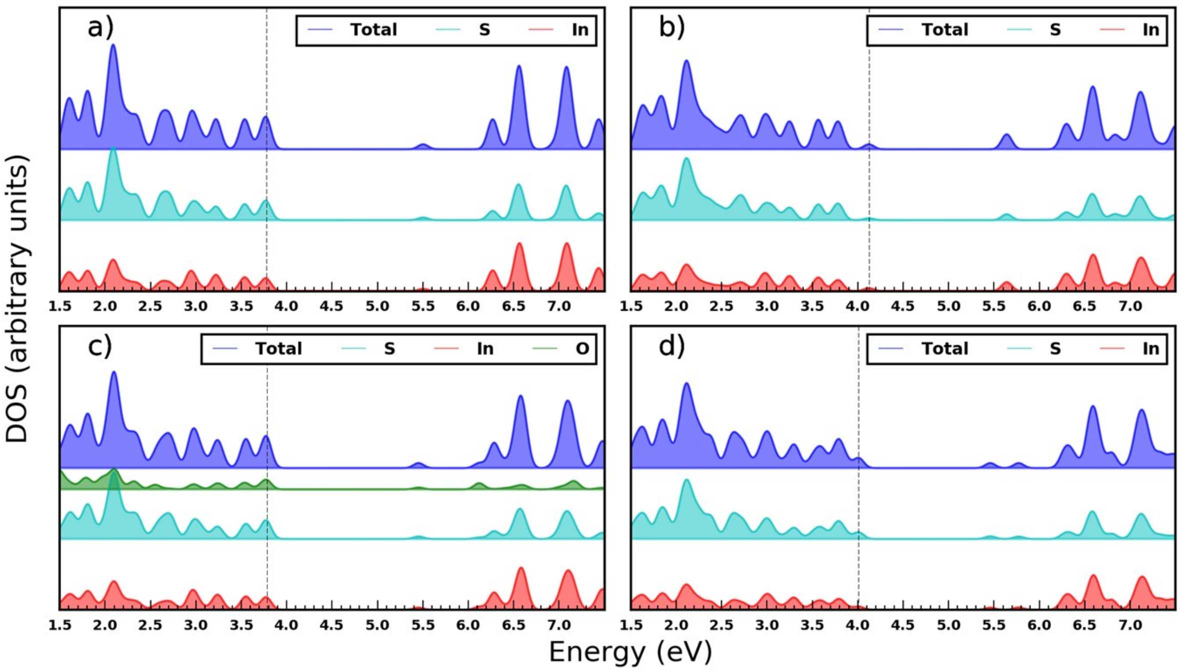

Figure S11: a) Shows the DOS for pristine InS with individual contributions. b) Shows the dos for InS with one Sulfur vacancy. c) Shows the DOS with Sulfur vacancy replaced by an oxygen atom. d) Shows the impact of an In vacancy on the DOS.

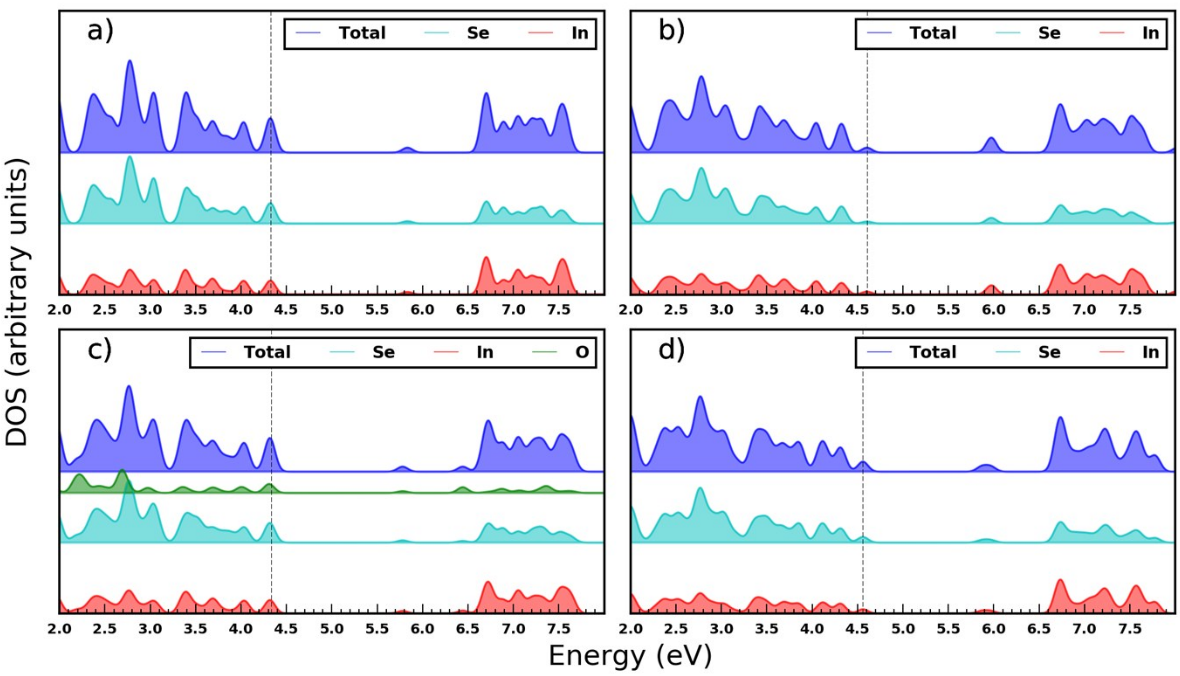

Figure S12: a) Shows the DOS for pristine InSe with individual contributions. b) Shows the dos for InSe with one Selenium vacancy. c) Shows the DOS with Selenium vacancy replaced by an oxygen atom. d) Shows the impact of an In vacancy on the DOS.

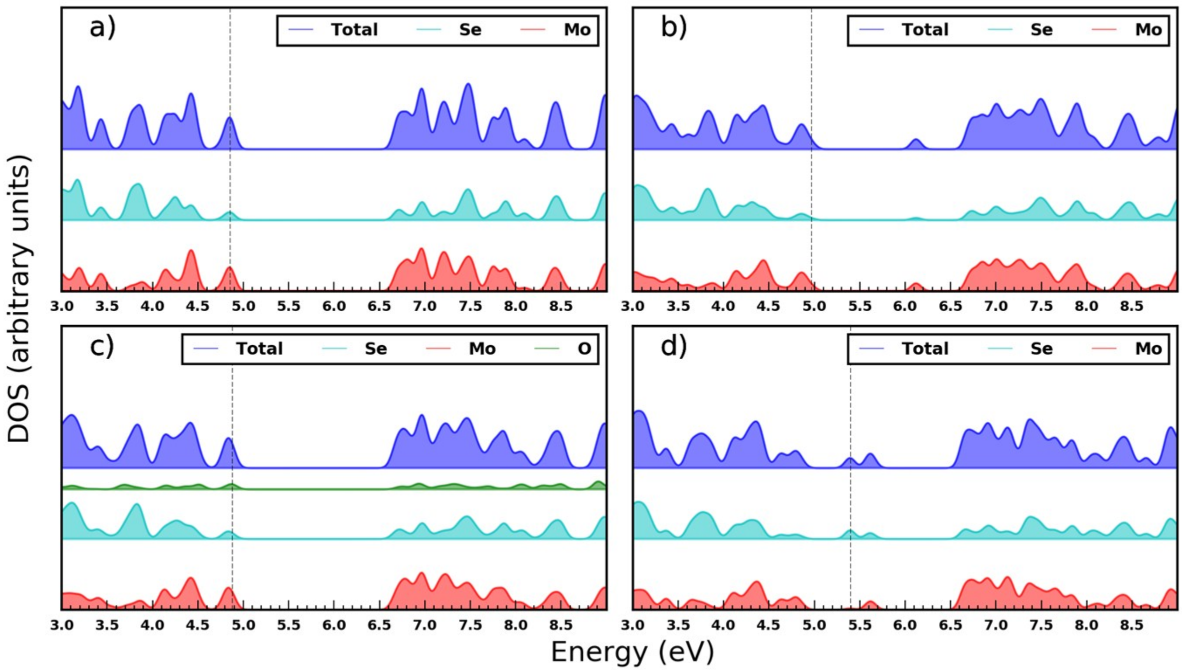

Figure S13: a) Shows the DOS for pristine $MoSe_2$-2H with individual contributions. b) Shows the dos for $MoSe_2$-2H with one Selenium vacancy. c) Shows the DOS with Selenium vacancy replaced by an oxygen atom. d) Shows the impact of an Mo vacancy on the DOS.

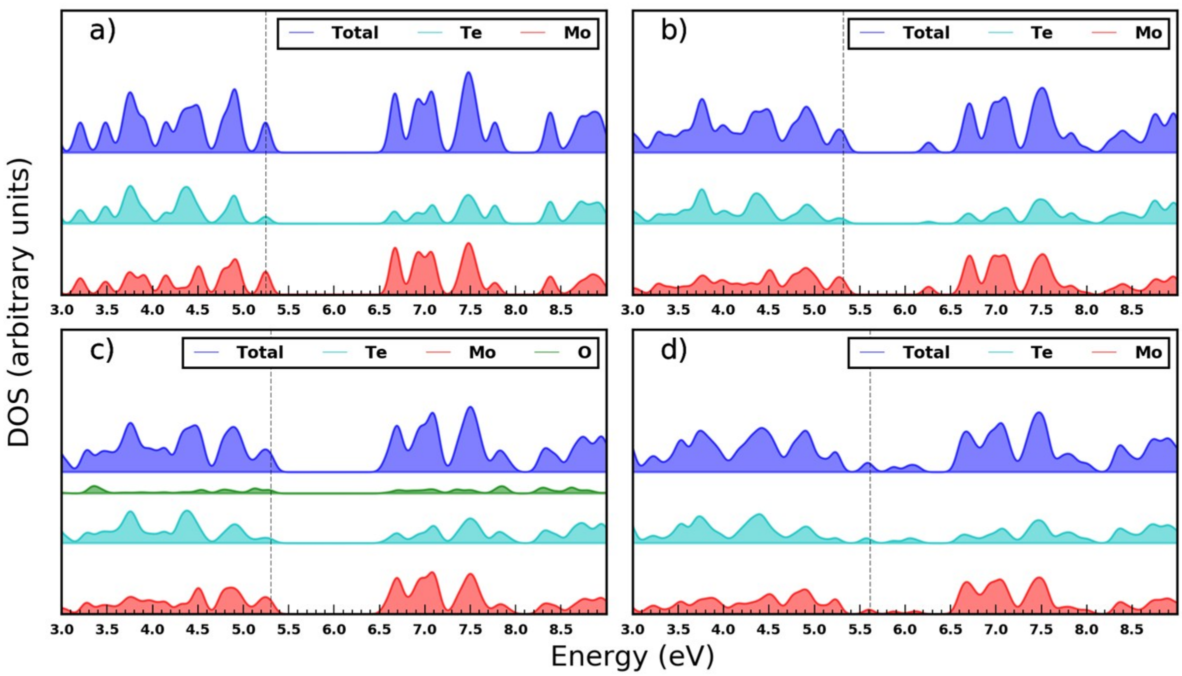

Figure S14: a) Shows the DOS for pristine $MoTe_2$-2H with individual contributions. b) Shows the dos for $MoTe_2$-2H with one Tellurium vacancy. c) Shows the DOS with Tellurium vacancy replaced by an oxygen atom. d) Shows the impact of an Mo vacancy on the DOS.

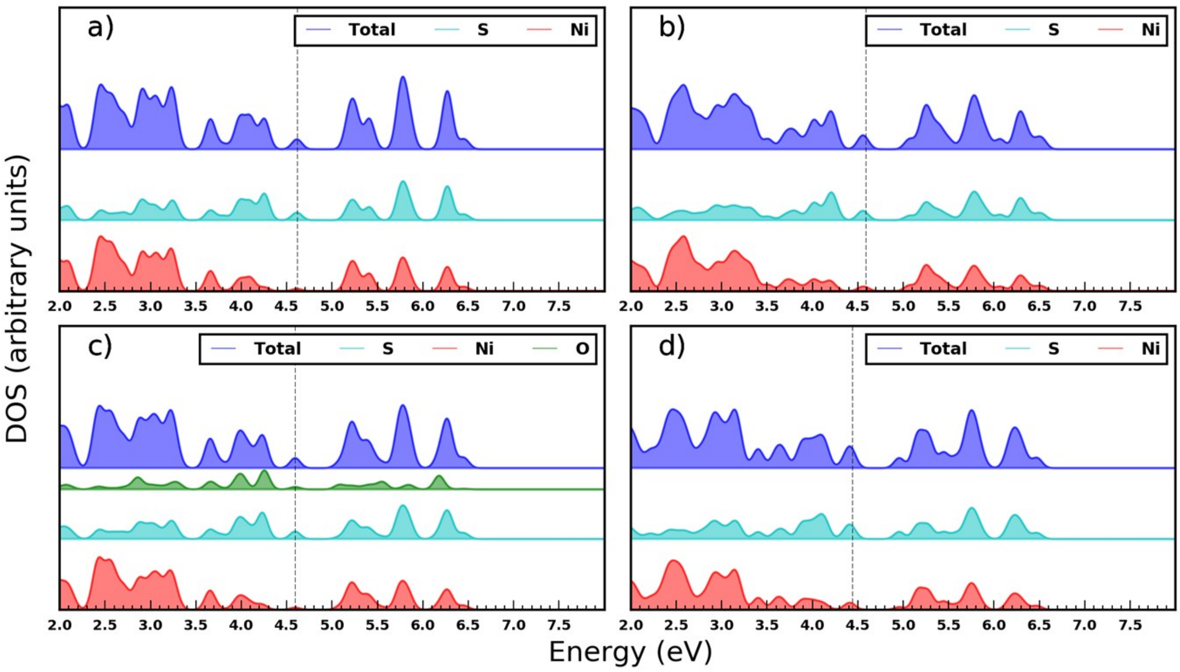

Figure S15: a) Shows the DOS for pristine NiS_2-1T with individual contributions. b) Shows the dos for NiS_2-1T with one Sulfur vacancy. c) Shows the DOS with Sulfur vacancy replaced by an oxygen atom. d) Shows the impact of an Ni vacancy on the DOS.

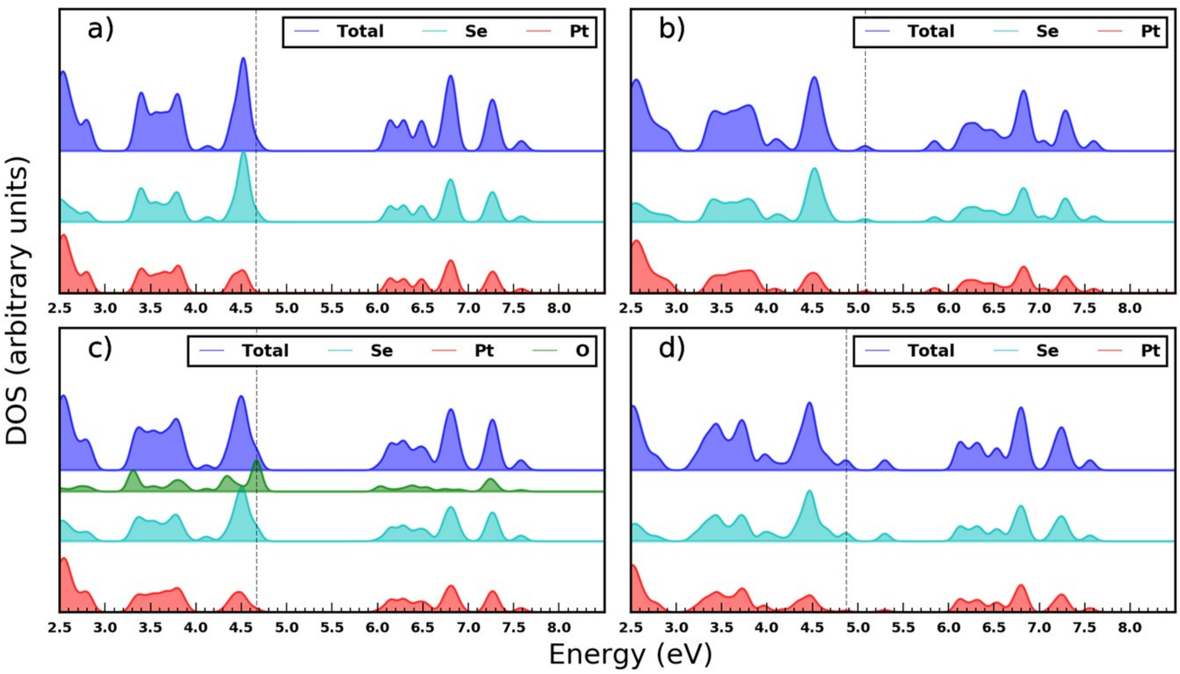

Figure S16: a) Shows the DOS for pristine $PtSe_2$-1T with individual contributions. b) Shows the dos for $PtSe_2$-1T with one Selenium vacancy. c) Shows the DOS with Selenium vacancy replaced by an oxygen atom. d) Shows the impact of an Pt vacancy on the DOS.

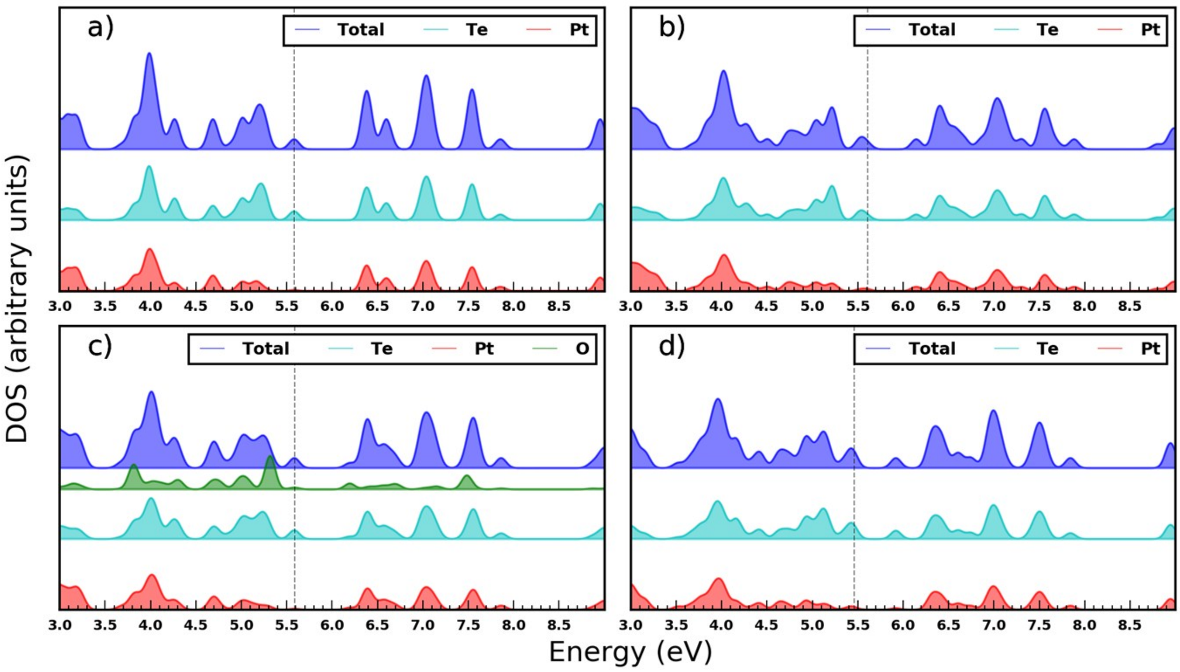

Figure S17: a) Shows the DOS for pristine $PtTe_2$-1T with individual contributions. b) Shows the dos for $PtTe_2$-1T with one Tellurium vacancy. c) Shows the DOS with Tellurium vacancy replaced by an oxygen atom. d) Shows the impact of an Pt vacancy on the DOS.

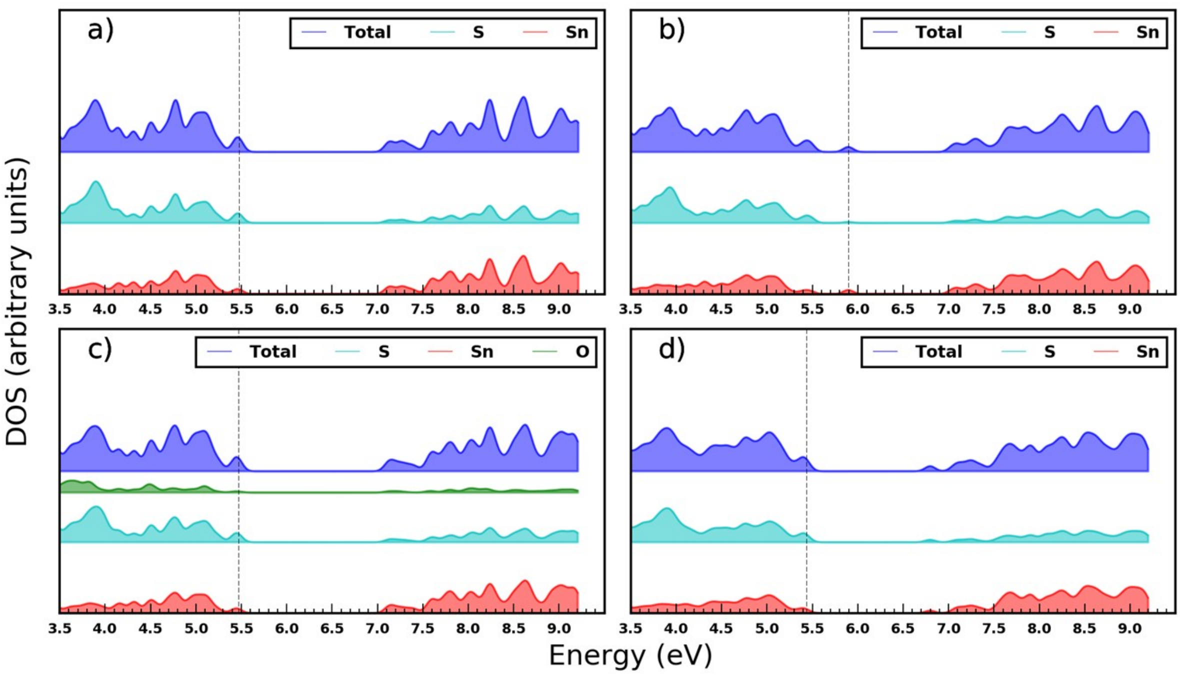

Figure S18: a) Shows the DOS for pristine SnS with individual contributions. b) Shows the dos for SnS with one Sulfur vacancy. c) Shows the DOS with Sulfur vacancy replaced by an oxygen atom. d) Shows the impact of an Sn vacancy on the DOS.

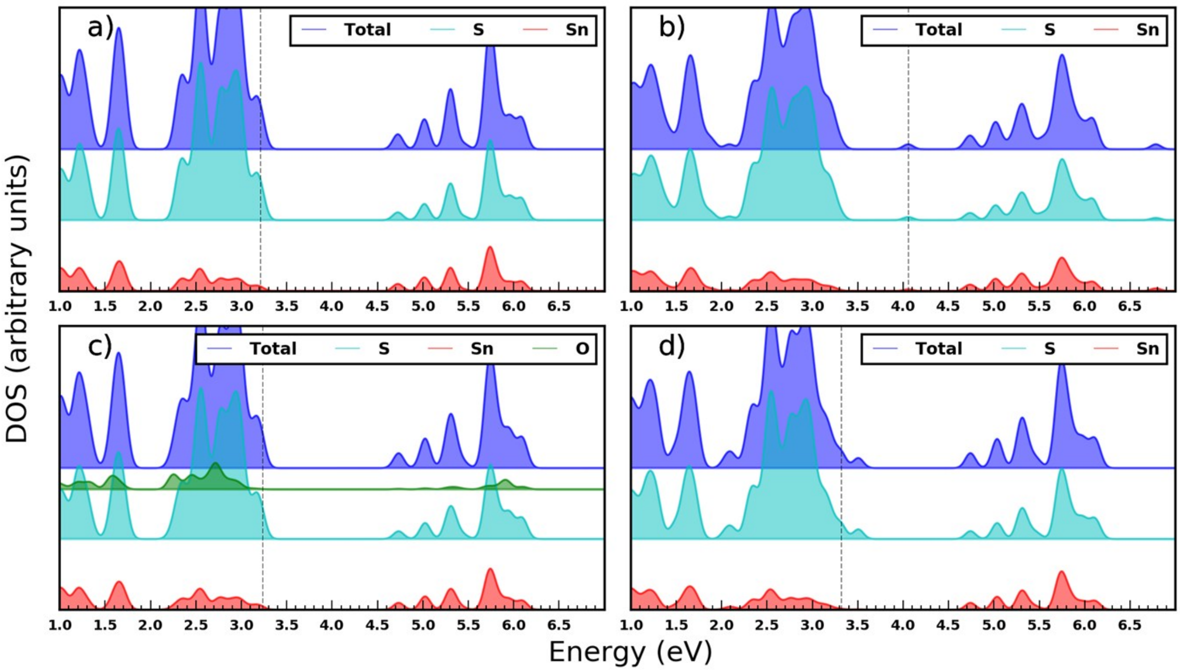

Figure S19: a) Shows the DOS for pristine SnS_2 with individual contributions. b) Shows the dos for SnS_2 with one Sulfur vacancy. c) Shows the DOS with Sulfur vacancy replaced by an oxygen atom. d) Shows the impact of an Sn vacancy on the DOS.

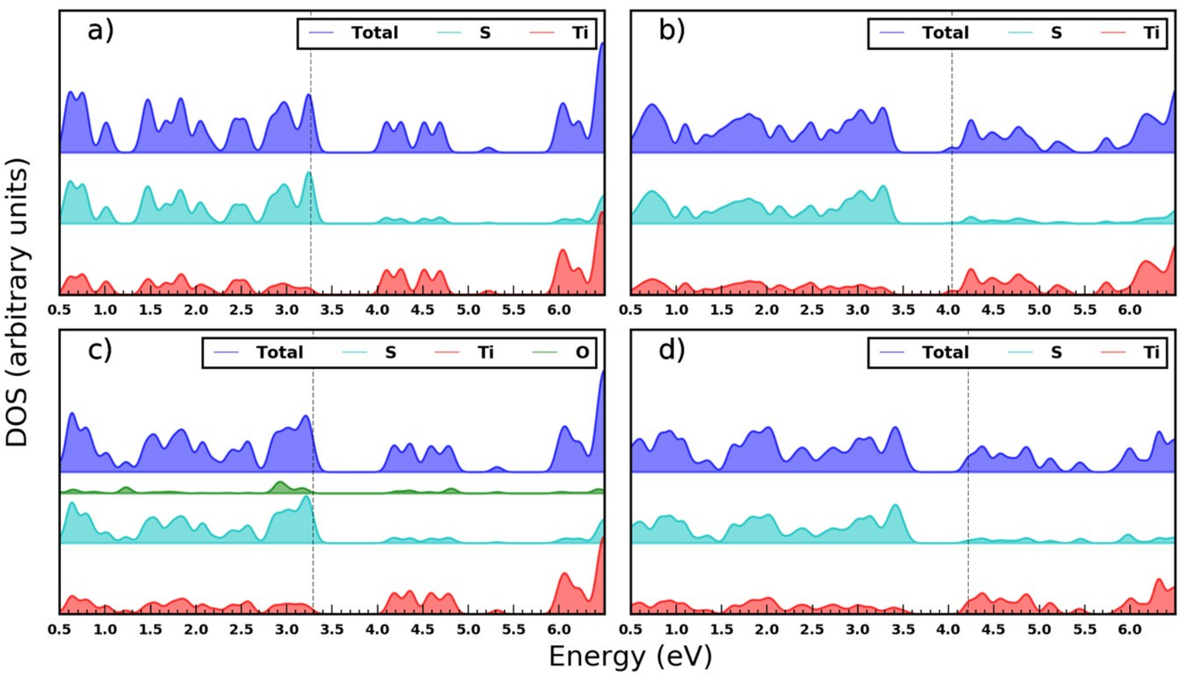

Figure S20: a) Shows the DOS for pristine TiS_2-2H with individual contributions. b) Shows the dos for TiS_2 with one Sulfur vacancy. c) Shows the DOS with Sulfur vacancy replaced by an oxygen atom. d) Shows the impact of an Ti vacancy on the DOS.

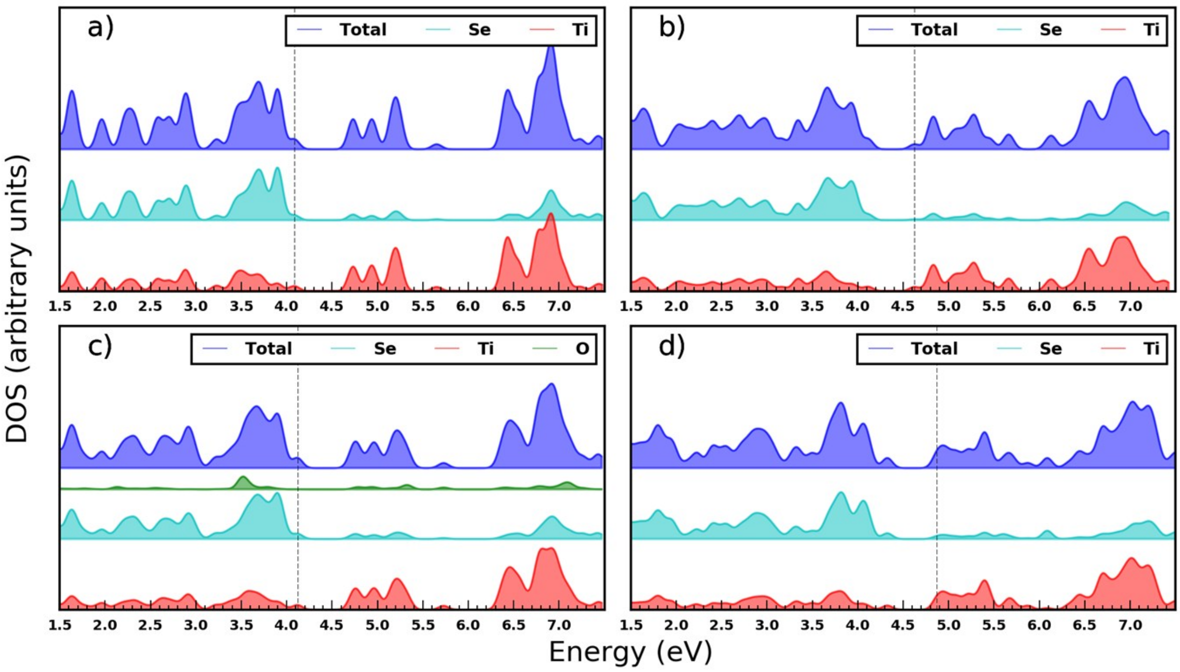

Figure S21: a) Shows the DOS for pristine $TiSe_2$-2H with individual contributions. b) Shows the dos for $TiSe_2$-2H with one Selenium vacancy. c) Shows the DOS with Selenium vacancy replaced by an oxygen atom. d) Shows the impact of a Ti vacancy on the DOS.

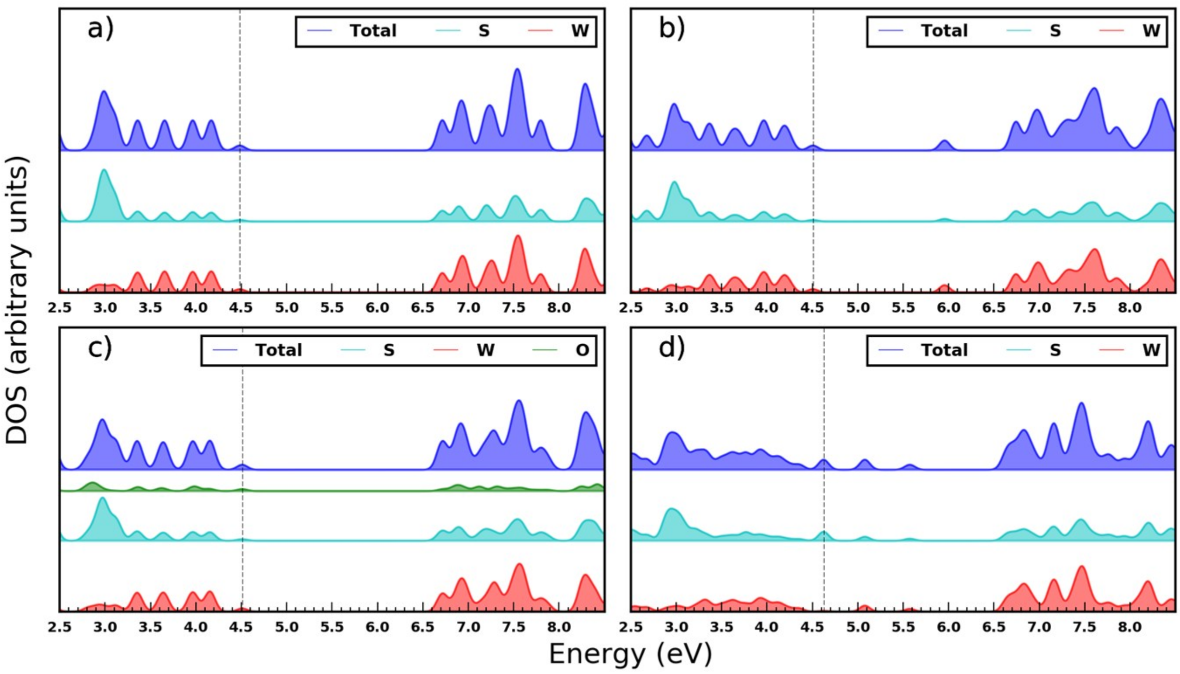

Figure S22: a) Shows the DOS for pristine WS_2-2H with individual contributions. b) Shows the dos for WS_2-2H with one Sulfur vacancy. c) Shows the DOS with Sulfur vacancy replaced by an oxygen atom. d) Shows the impact of a W vacancy on the DOS.

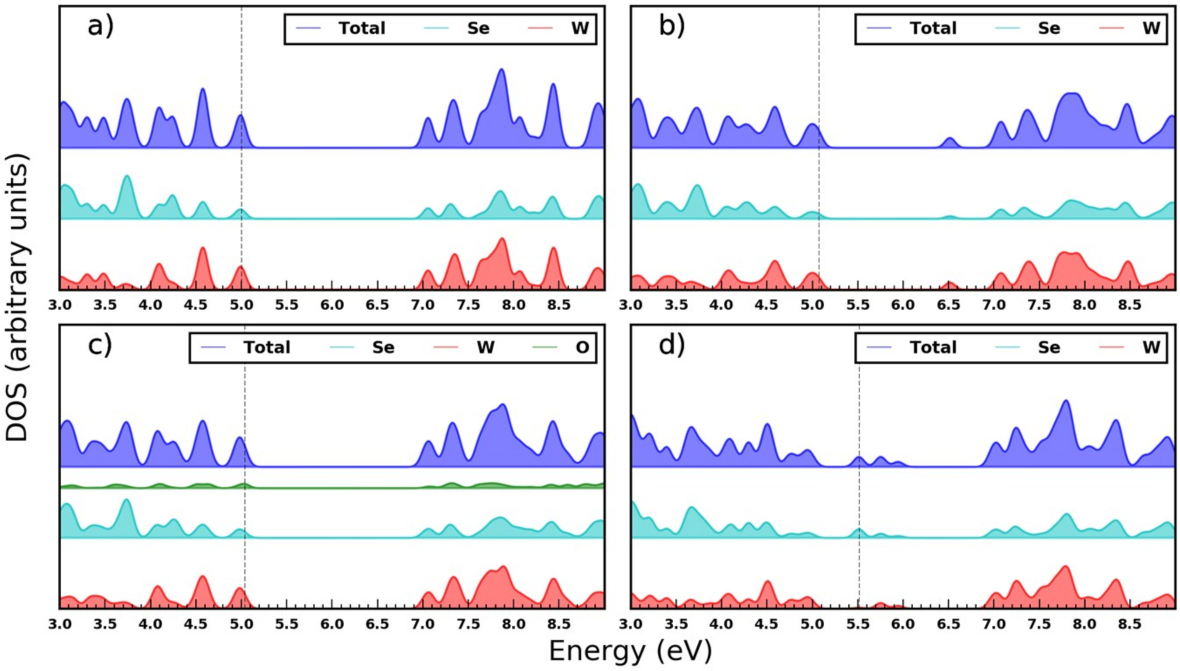

Figure S23: a) Shows the DOS for pristine WSe_2-2H with individual contributions. b) Shows the dos for WSe_2-2H with one Selenium vacancy. c) Shows the DOS with Selenium vacancy replaced by an oxygen atom. d) Shows the impact of a W vacancy on the DOS.

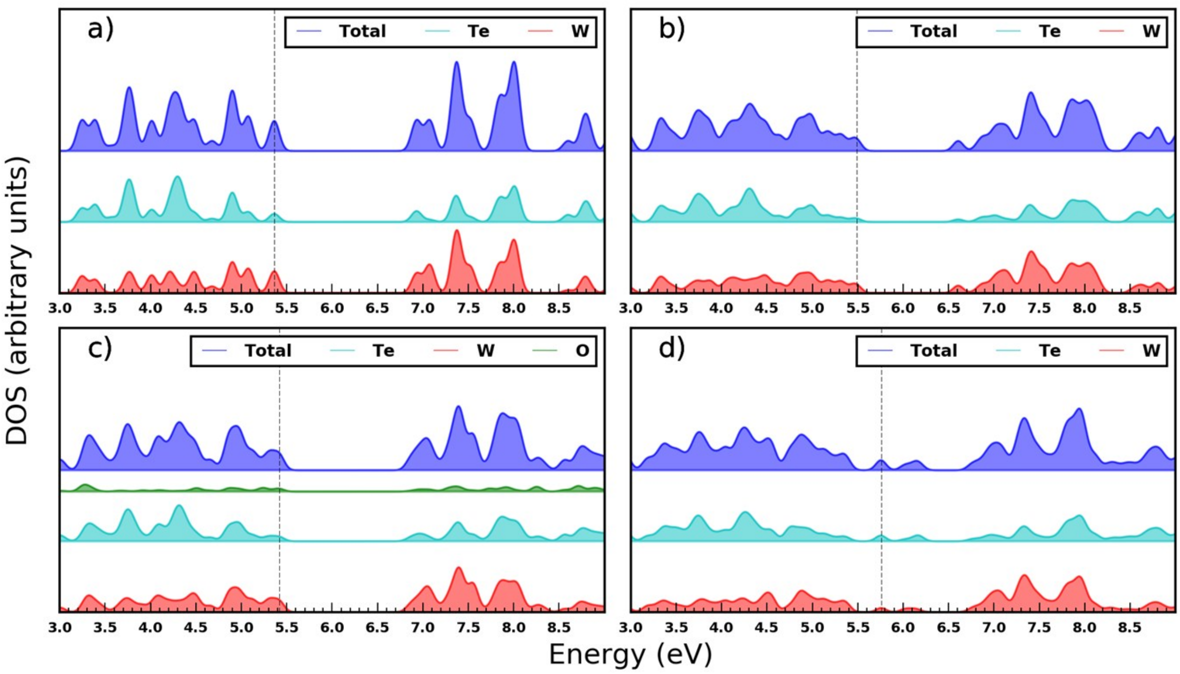

Figure S24: a) Shows the DOS for pristine WTe_2-2H with individual contributions. b) Shows the dos for WTe_2-2H with one Tellurium vacancy. c) Shows the DOS with Tellurium vacancy replaced by an oxygen atom. d) Shows the impact of a W vacancy on the DOS.

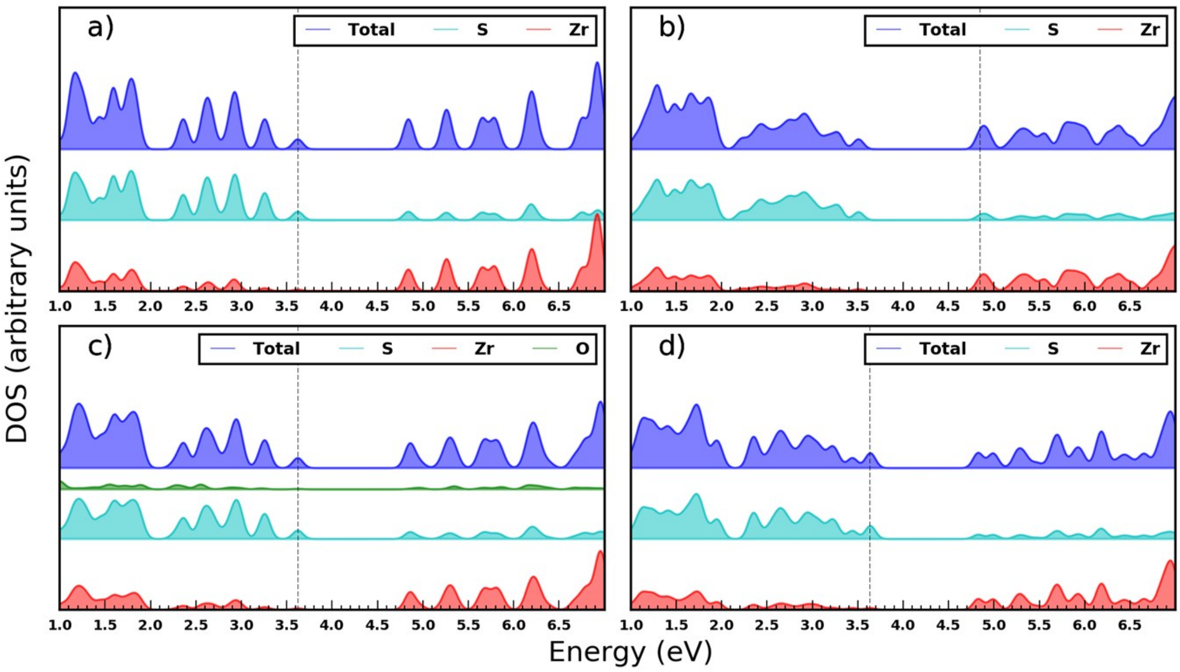

Figure S25: a) Shows the DOS for pristine ZrS_2-1T with individual contributions. b) Shows the dos for ZrS_2-1T with one Sulfur vacancy. c) Shows the DOS with Sulfur vacancy replaced by an oxygen atom. d) Shows the impact of a Zr vacancy on the DOS.

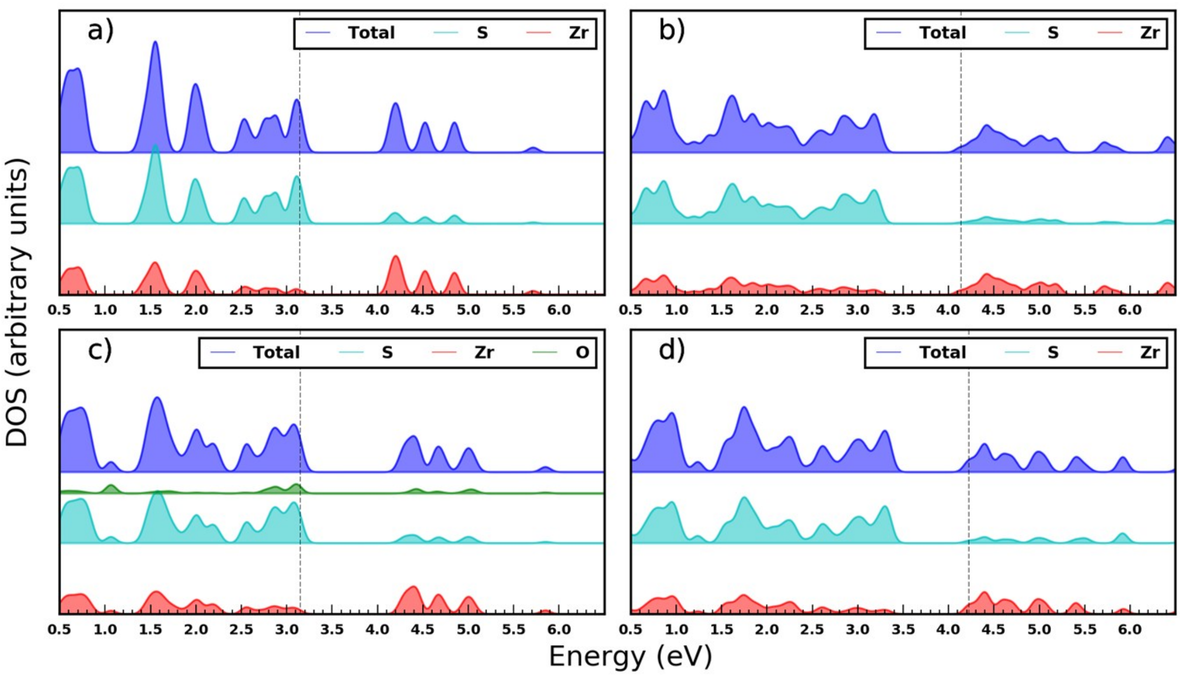

Figure S26: a) Shows the DOS for pristine ZrS_2-2H with individual contributions. b) Shows the dos for ZrS_2-2H with one Sulfur vacancy. c) Shows the DOS with Sulfur vacancy replaced by an oxygen atom. d) Shows the impact of a Zr vacancy on the DOS.

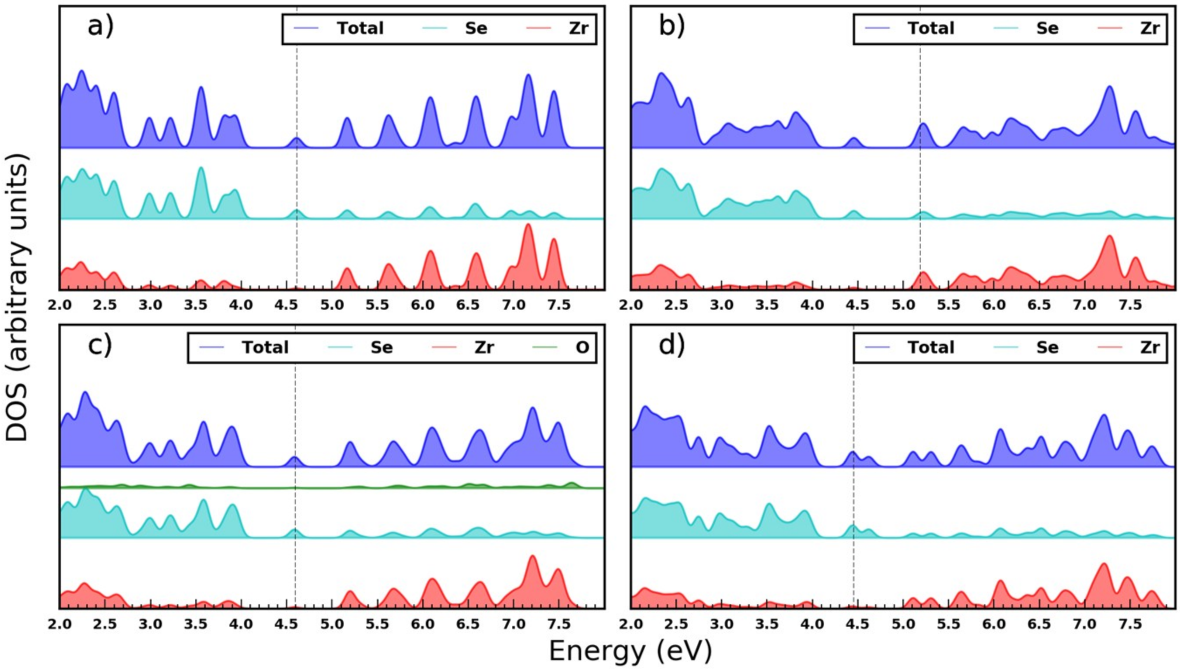

Figure S27: a) Shows the DOS for pristine $ZrSe_2$-1T with individual contributions. b) Shows the dos for $ZrSe_2$-1T with one Selenium vacancy. c) Shows the DOS with Selenium vacancy replaced by an oxygen atom. d) Shows the impact of a Zr vacancy on the DOS.

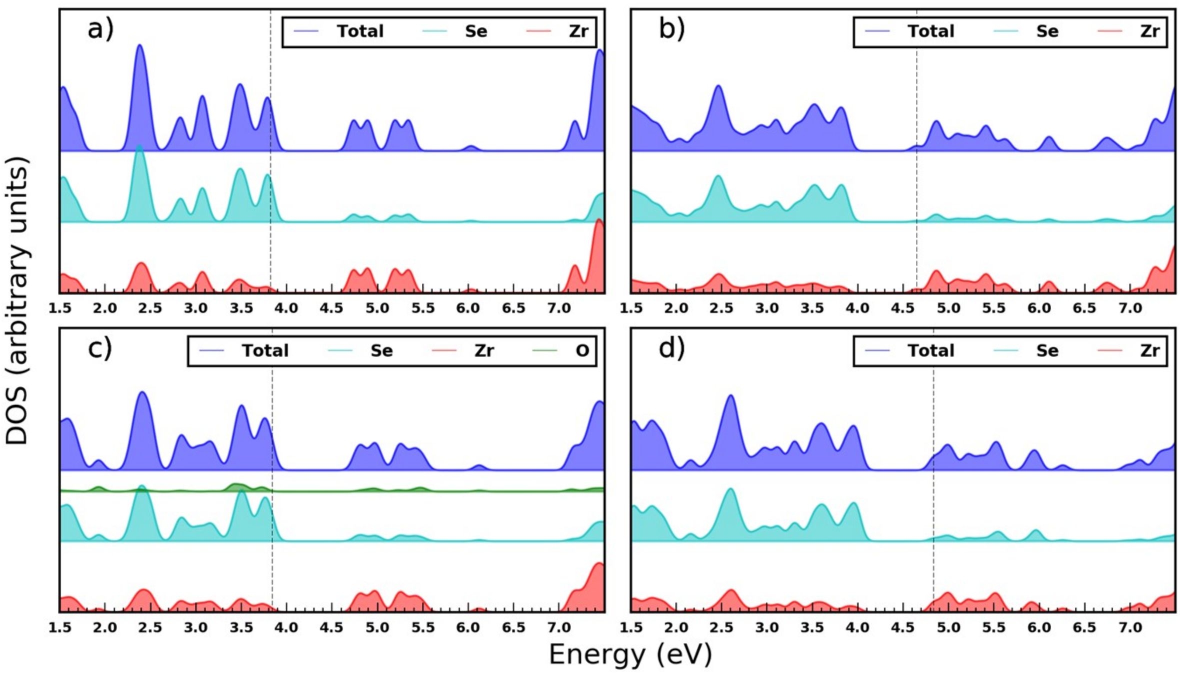

Figure S28: a) Shows the DOS for pristine $ZrSe_2$-2H with individual contributions. b) Shows the dos for $ZrSe_2$-2H with one Selenium vacancy. c) Shows the DOS with Selenium vacancy replaced by an oxygen atom. d) Shows the impact of a Zr vacancy on the DOS.

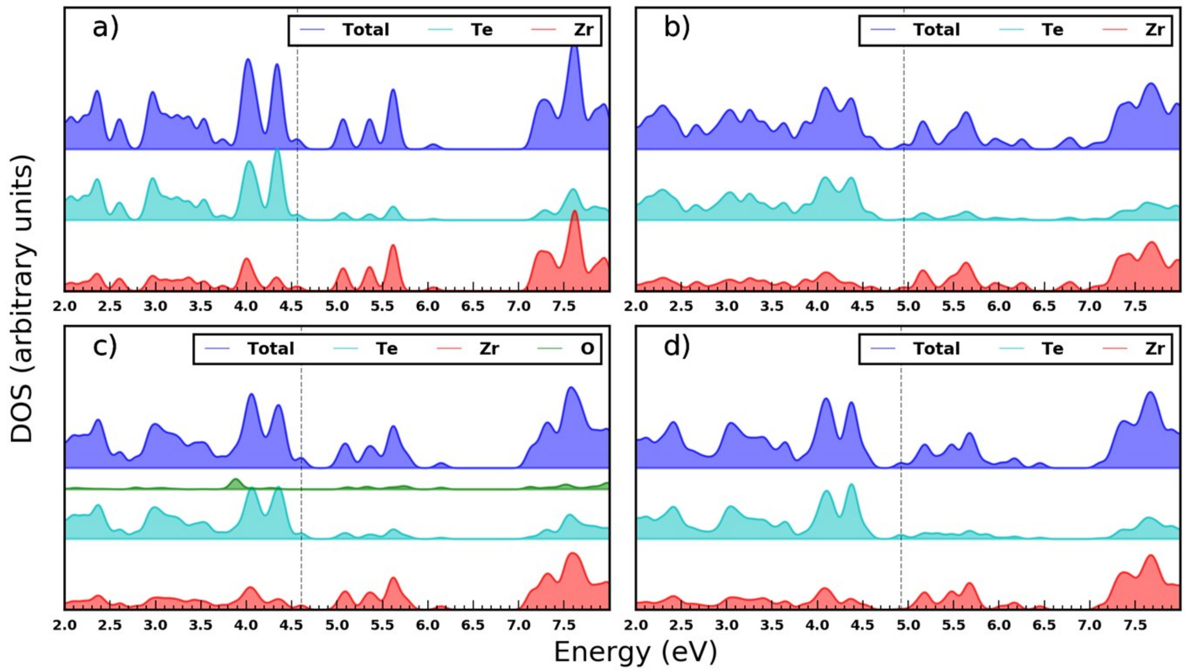

Figure S29: a) Shows the DOS for pristine $ZrTe_2$-2H with individual contributions. b) Shows the dos for $ZrTe_2$-2H with one Tellurium vacancy. c) Shows the DOS with Tellurium vacancy replaced by an oxygen atom. d) Shows the impact of a Zr vacancy on the DOS.

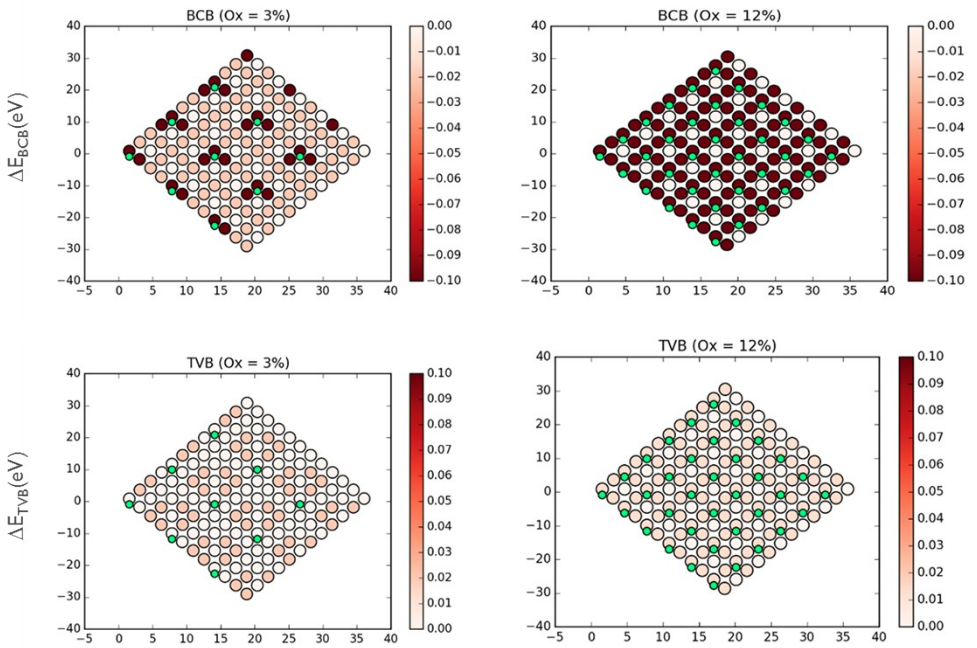

Figure S30: Change in the bottom of the conduction band (BCB) (top figures) and top of the valence band (TVB)(bottom figures) of a MoS_2 supercell for two different concentrations of oxygen. A higher impact on BCB can be seen as compared to TVB.