Electronic Supplementary Material (ESI) for RSC Advances.

SUPPORTING INFORMATION

Atomistic insight into the oxidation of monolayer transition metal dichalcogenides: from structures to electronic properties

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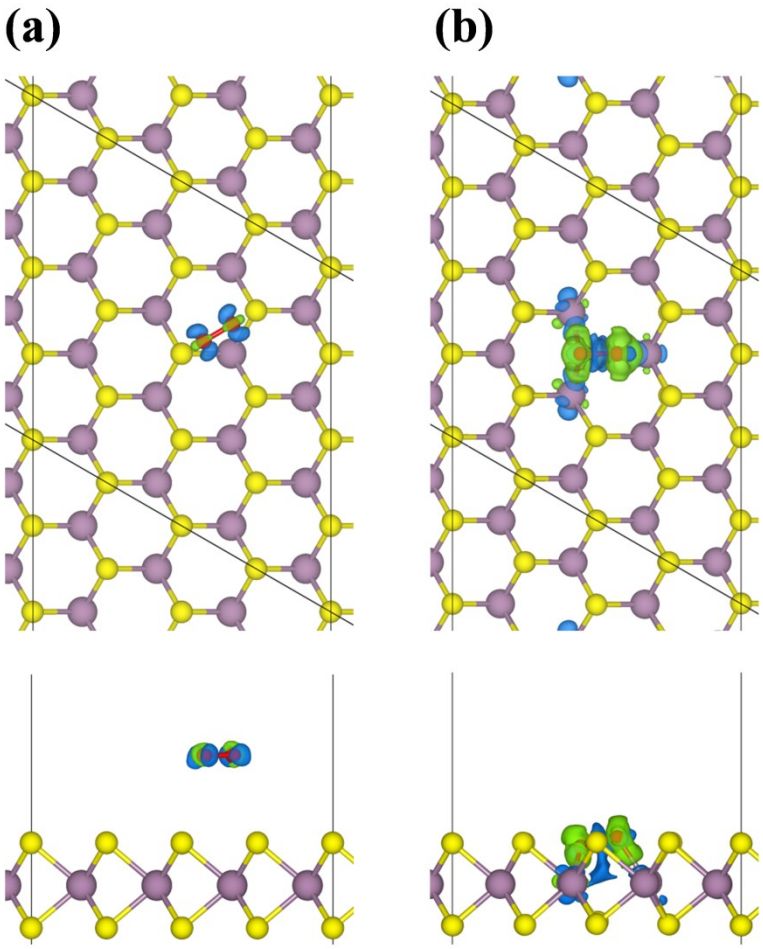

Figure S1. Charge density difference for O_2 adsorbed on (a) perfect and (b) defective MoS_2 monolayer. The iso-surface for electron density is 2×10^{-4} e/Å^3 for (a) and 6×10^{-3} e/Å^3 for (b). Green is charge accumulation and blue is charge depletion. The charge density difference is calcluated as $Charge_{total} - Charge_{O2} - Charge_{sub}$, where $Charge_{total}$ is the total charge density of the systems, $Charge_{O2}$ is the charge density of O_2 and $Charge_{sub}$ is the charge density of perfect or defective MoS_2 monolayer.

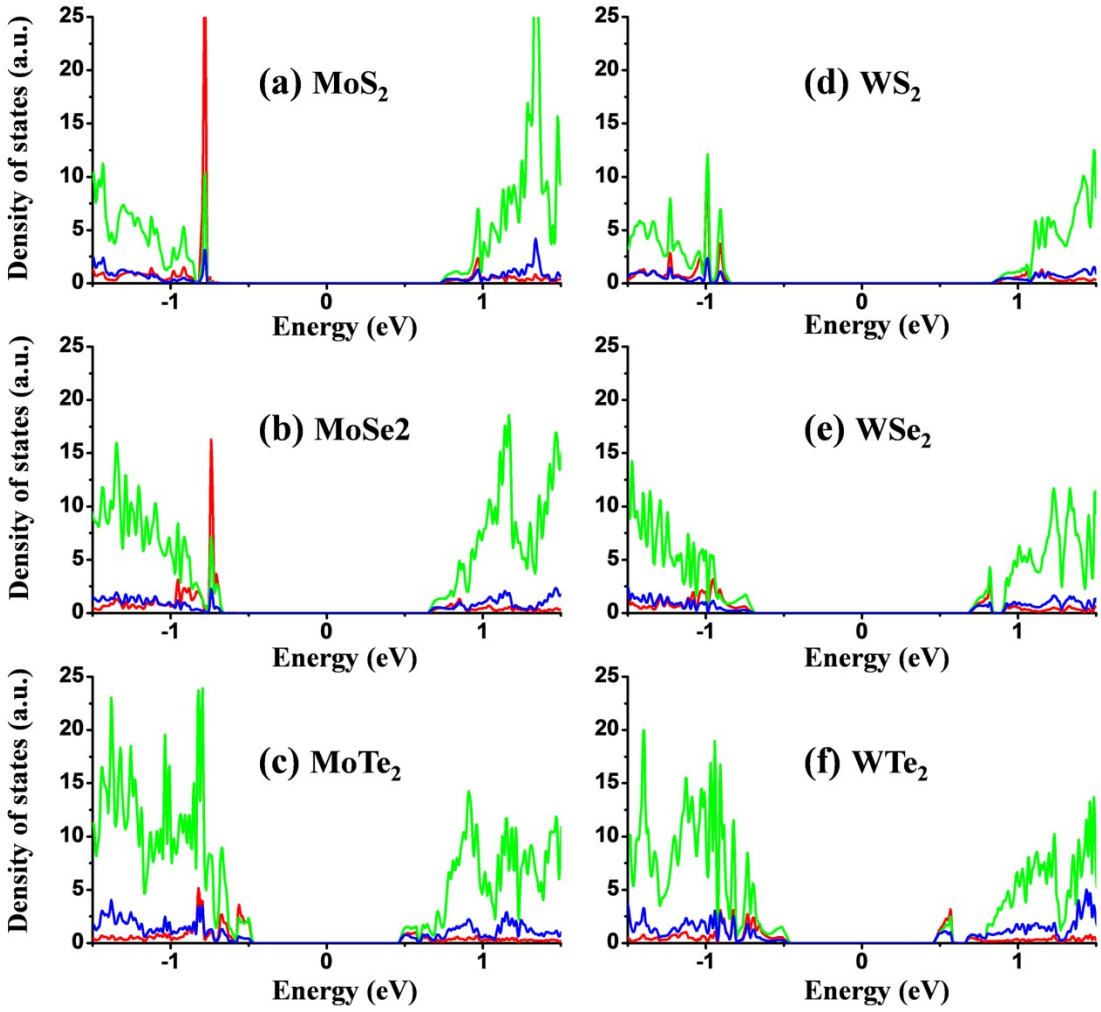

Figure S2. Partial density of states (PDOS) for all the six defective TMD monolayers with O_2 adsorption at vacancy sites. Red lines represent states from O_2. Green lines represent states from chalcogen (S, Se or Te). Blue lines represent states from transition metal atoms.