Electronic Supplementary Information

First-principles study of the oxidation susceptibility of WS_2, WSe_2, and WTe_2 monolayers

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1. Pristine WX_2 monolayers

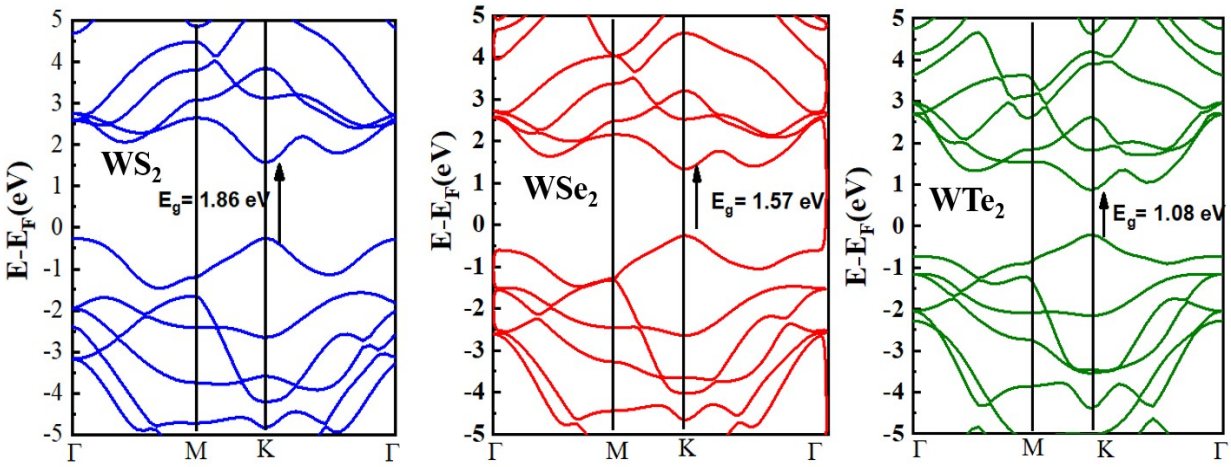

Figure S1. Band Structure of pristine WX_2 monolayers

2. O_2 and O_3 molecules

Table S1 Bond Lengths and Bond Angles for the O_2 and O_3 molecules

Molecule	$R_{O\text{-}O}$ (O_2)	$R_{O\text{-}O}$ (O_3)	$A_{O\text{-}O\text{-}O}$ (O_3)
Bond-Length ($R_{O\text{-}O}$)/ Bond Angle ($A_{O\text{-}O\text{-}O}$)	1.24 Å	1.28 Å	118.15°
	1.24 Å (DFT)[41] 1.21 Å (expt.)[42]	1.28 Å (expt.)[43] 1.28 Å (DFT)[44]	116. 49° (expt.)[43] 117.90° (DFT)[44]

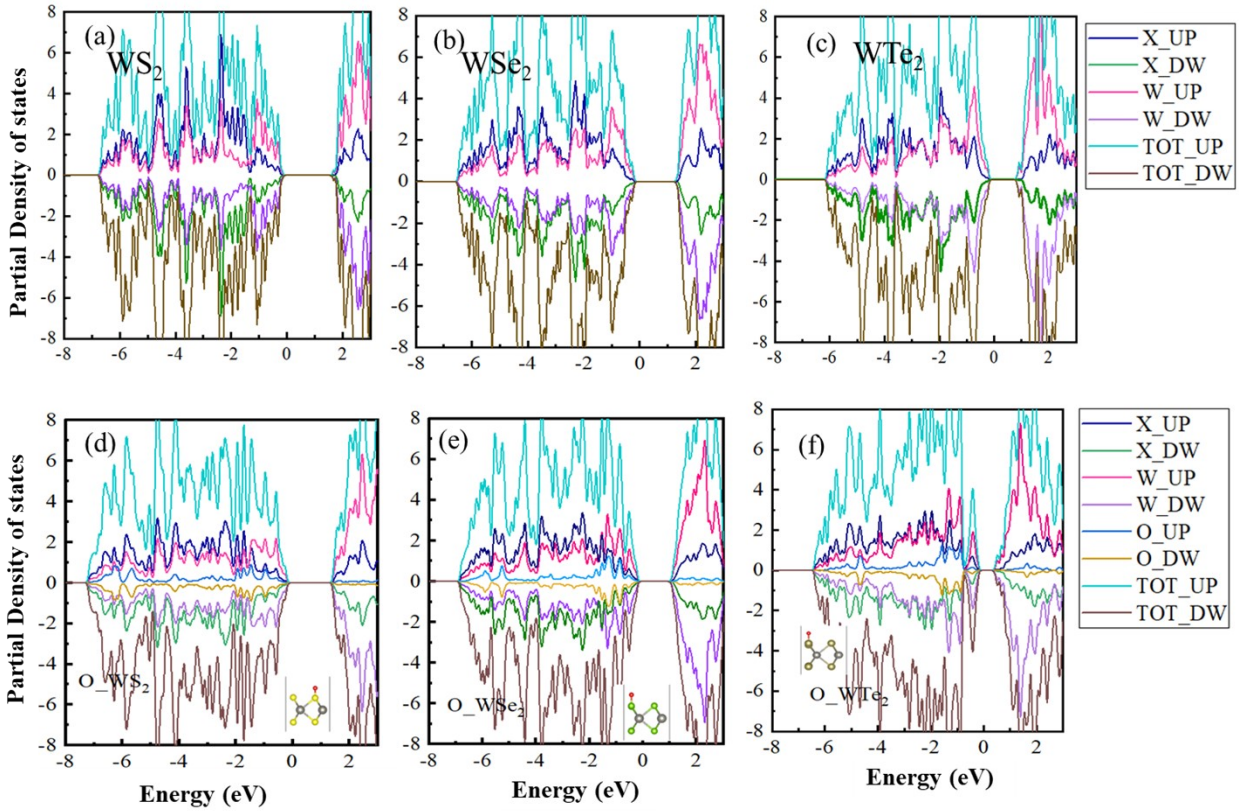

Figure S2. Calculated Total DOS and PDOS for (a)-(c) pristine and (d)-(f) oxygen adsorbed WX_2 monolayers.