SUPPORTING INFORMATION:

Table S1: Lattice constants, M-X bond length, X-M-X bond angles and bandgap without (E_g (eV)) and with spin orbit coupling (E_g (eV)_SO) in an orthorhombic supercell.

SYSTEMS	a (Å)	b (Å)	$d_{M\text{-}X}$ (Å)	Θ°	E_g (eV)	E_g (eV)_SO
MoS_2	3.18	5.51	2.41	82.52	1.67	1.59
$MoSe_2$	3.31	5.74	2.54	81.52	1.44	1.34
$MoTe_2$	3.55	6.15	2.73	81.06	1.08	0.94
WS_2	3.18	5.51	2.42	82.33	1.82	1.55
WSe_2	3.32	5.74	2.54	81.30	1.55	1.25
WTe_2	3.55	6.15	2.74	80.96	1.06	0.74

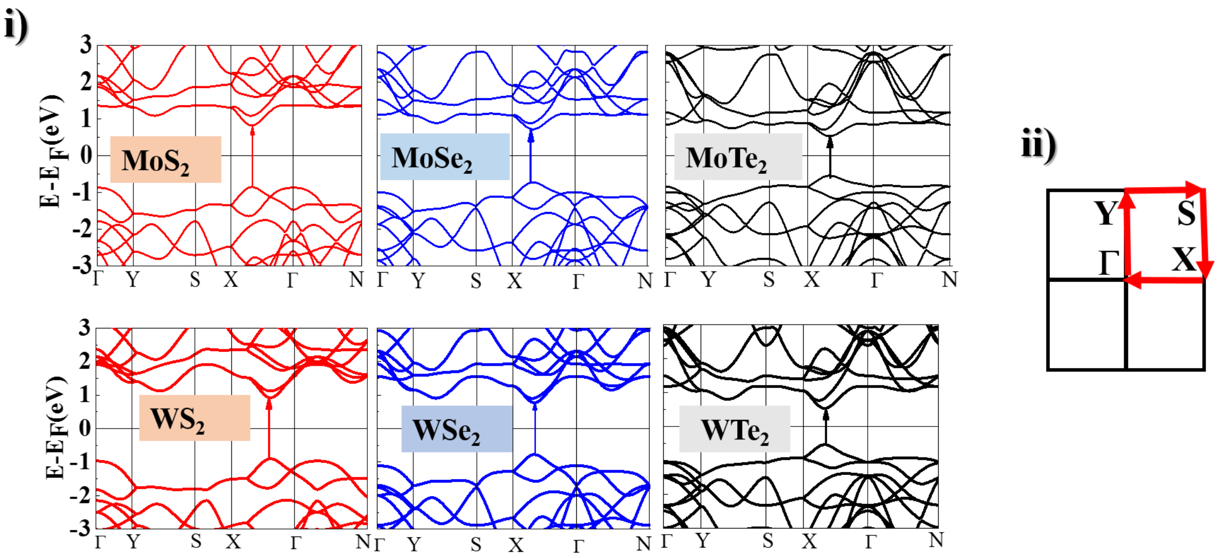


Figure S1 i) Band structures ii) K-path for the orthorhombic supercell.

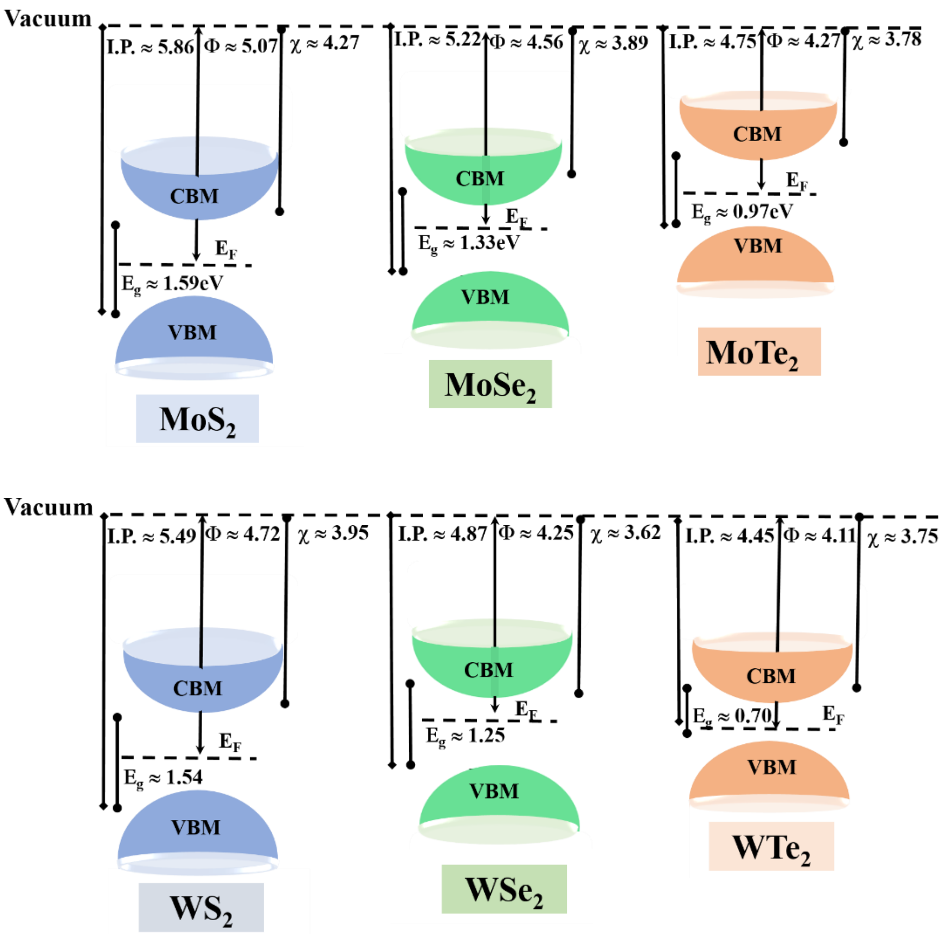


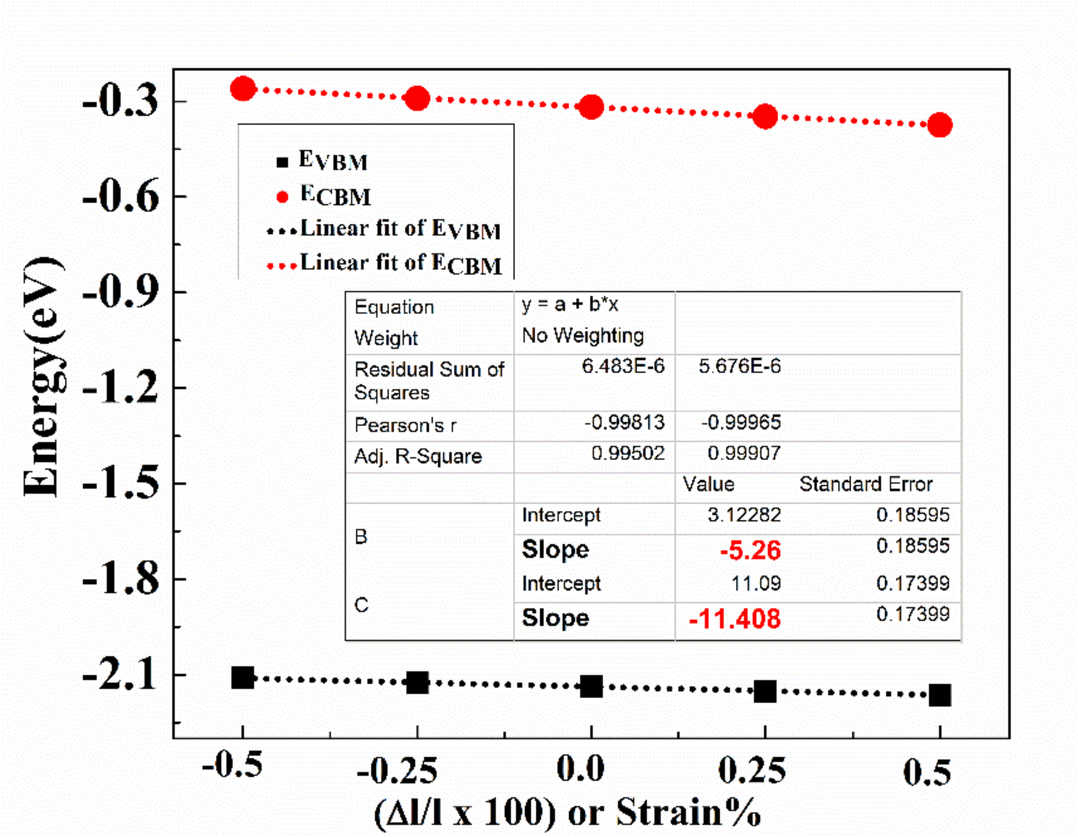
Figure S2. Ionisation Potential (I.P.), Work Function (Φ), electron affinity (χ), Band gap of the TMDCs for the six-single layer transition metal dichalcogenides with spin orbit coupling. All values mentioned above are in eV.

Table S2 Carrier effective masses for hexagonal supercell in units of the rest mass of electron (x and y are respectively the zig-zag and the arm-chair directions respectively).

Systems	**$m_{h\_x}(m_0)$**	**$m_{h\_y}(m_0)$**	**$m_{e\_x}(m_0)$**	**$m_{h\_y}(m_0)$**
MoS_2	0.567	0.567	0.469	0.469
$MoSe_2$	0.647	0.647	0.545	0.545
$MoTe_2$	0.693	0.693	0.575	0.575
WS_2	0.412	0.412	0.309	0.309
WSe_2	0.454	0.454	0.340	0.336
WTe_2	0.400	0.400	0.302	0.299

Deformation Potential:

In calculations for charge carrier mobility, the deformation potential is obtained from the slope of the band edges with an infinitesimal magnitude of applied strain uniaxially. The slope of the conduction and valence band edge with small strain gives the deformation potential for the electrons and holes respectively. The deformation potential for WS_2 for holes and electrons along the zig-zag direction are provided below. A similar approach can be applied to the other systems as well.



Equation	y = a + b*x		
Weight	No Weighting		
Residual Sum of Squares	6.483E-6	5.676E-6	
Pearson's r	-0.99813	-0.99965	
Adj. R-Square	0.99502	0.99907	
		Value	Standard Error
B	Intercept	3.12282	0.18595
	Slope	**-5.26**	0.18595
C	Intercept	11.09	0.17399
	Slope	**-11.408**	0.17399

Figure S3. Deformation Potential (DP) along the zig-zag direction in single layer WS_2, where E_{CBM} and E_{VBM} are the energies of the conduction band minimum and the valence band maximum respectively. Slope of E_{CMB} and E_{VBM} with strain gives the DP for electrons and holes along the zig-zag direction

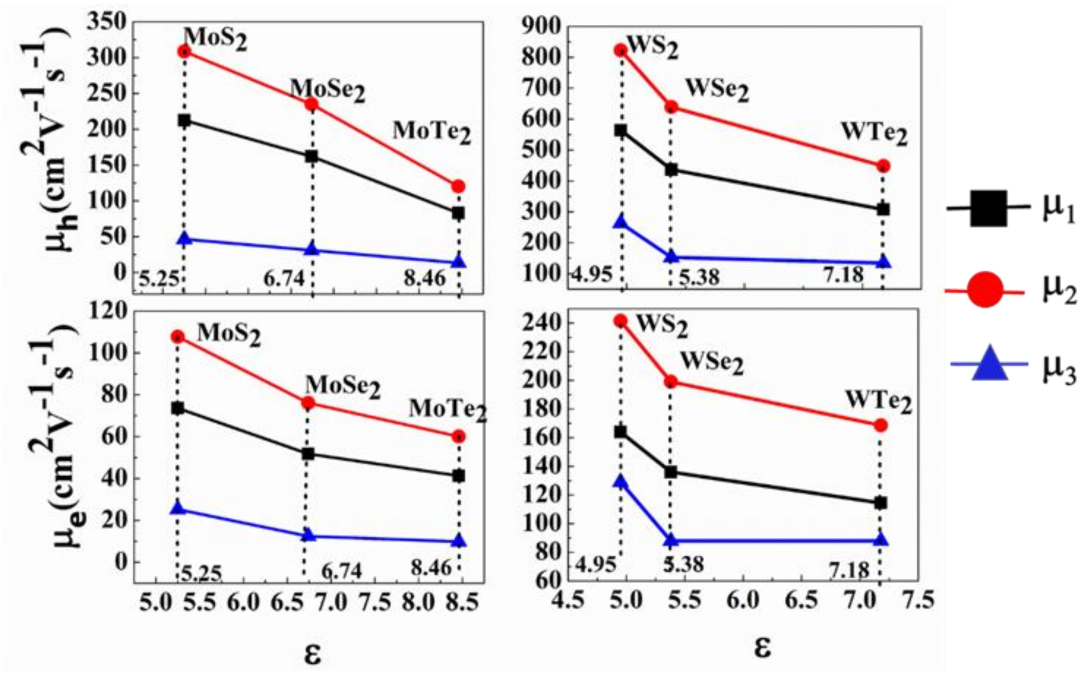


Figure S4. Variation in the mobility (along the armchair direction) with the macroscopic static dielectric constants for all six TMDC monolayers.

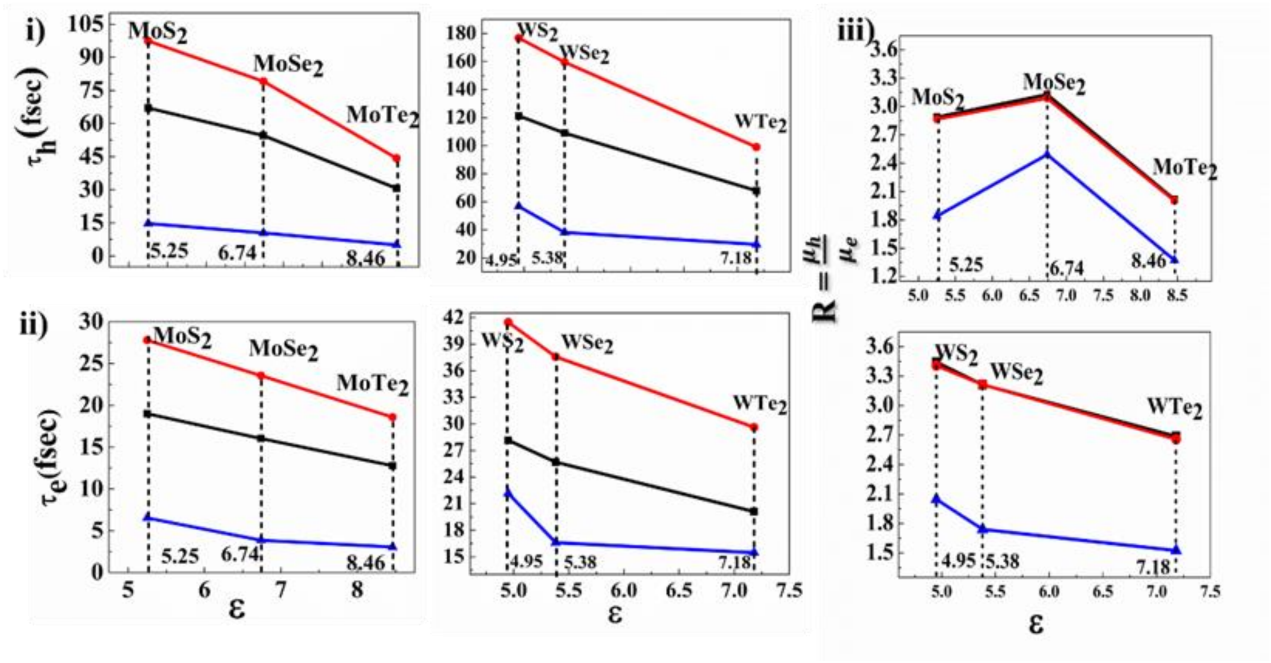


Figure S5. i) Electron Relaxation time ii) Hole Relaxation time for the six TMDC monolayers with the static macroscopic dielectric constant along the arm-chair direction iii) carrier mobility ratio, $R = \frac{\mu_h}{\mu_e}$, along the arm-chair direction.

Table S3. Electron Mobility along the armchair direction solely based on piezoelectric effects.

Systems	e_{11} (10^{-10}) C/m	D_{pz} (eV)	μ_{PZ} ($cm^2V^{-1}s^{-1}$)
MoS_2	3.35	5.13	107.76
$MoSe_2$	3.79	4.48	57.47
$MoTe_2$	4.61	4.34	49.32
WS_2	2.44	3.93	1136.83
WSe_2	2.52	3.74	697.03
WTe_2	3.10	3.44	831.37

Table S4. Total Electron Mobility along the armchair direction.

Systems	μ_{PZ} ($cm^2V^{-1}s^{-1}$)	μ_{LA} ($cm^2V^{-1}s^{-1}$)	μ_T ($cm^2V^{-1}s^{-1}$)
MoS_2	107.76	25.28	20.47
$MoSe_2$	57.47	11.45	9.54
$MoTe_2$	49.32	9.87	8.22
WS_2	1136.83	128.99	115.85
WSe_2	697.03	87.94	78.09
WTe_2	831.37	87.97	79.55

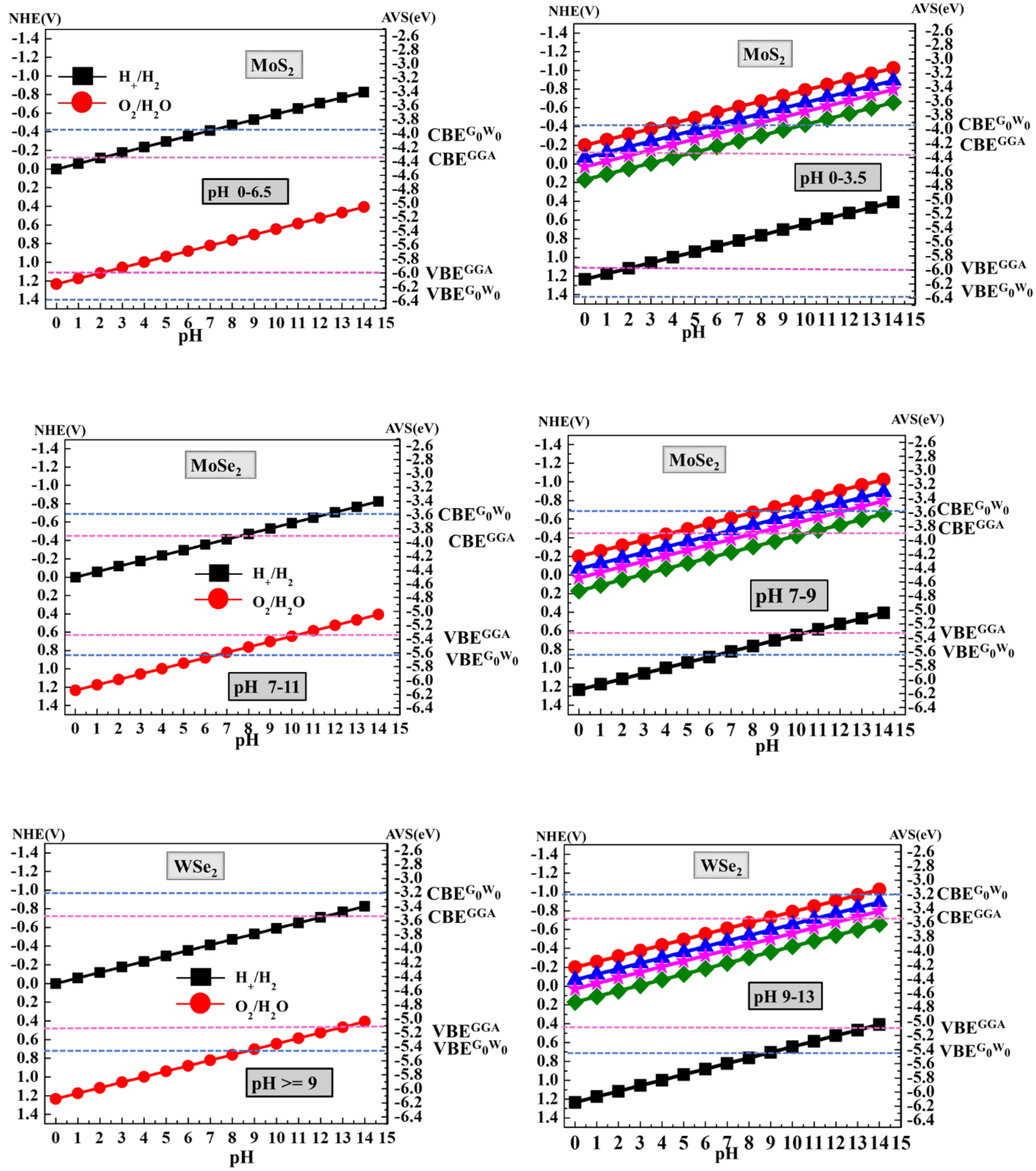


Figure S6. Variation in band edges in single layer TMDCs with redox potentials for (i) water splitting and (ii) CO_2 photoreduction with respect to AVS (eV) or NHE (V), which are acronyms for absolute vacuum scale and the normal hydrogen electrode respectively (suitable pH range have been shown as Figure insets). Also, the band edges calculated using GGA and G_0W_0 have been indicated alongside.

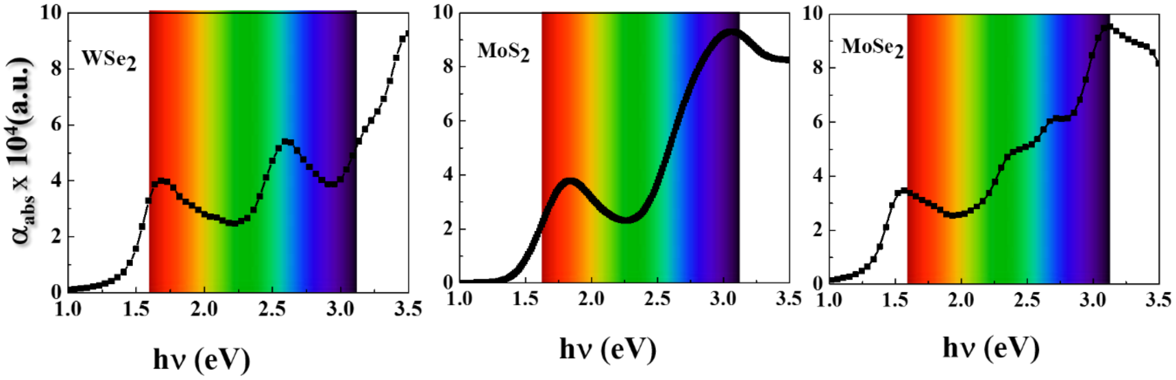


Figure S7. Optical absorbance for WSe$_2$, MoS$_2$ and MoSe$_2$ monolayers.